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1974 J. Phys. A: Math. Nucl. Gen. 7 807

(http://iopscience.iop.org/0301-0015/7/7/007)

J. Phys. A: Math., Nucl. Gen., Vol. 7, No. 7, 1974. Printed in Great Britain. © 1974

The splitting of a degenerate level under the action of a symmetry-breaking hamiltonian

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Received 3 September 1973, in final form 29 October 1973

Abstract. Recently Biedenharn and Gamba described a simple group-theoretical method to calculate the quantitative splitting of a degenerate energy level under the action of a symmetry-breaking hamiltonian. In this paper we provide the general proofs for the rules of the method and clarify the group-theoretical background. Furthermore we discuss the various kinds of multiplicities which can arise and the difficulties which they entail.

1. Introduction

The quantitative problem of the splitting of a degenerate level under the action of a symmetry-breaking hamiltonian was recently discussed by Biedenharn and Gamba (1972). They presented a method to solve this problem in an elegant way, which is shorter and simpler than the more conventional methods (cf for example Judd 1963). In these conventional methods one first of all has to calculate a number of matrix elements of the perturbation hamiltonian (either by applying the Wigner–Eckart theorem or by using an operator equivalent approach, see Judd (1963) and Stevens (1952)) and then one has to solve a secular equation. The most important advantages of the method discussed by Biedenharn and Gamba (1972) are that one does not need any Clebsch–Gordan coefficient and that it is not necessary to solve a secular equation. The fact that Clebsch–Gordan coefficients (or operator equivalents) are not required implies that the method of Biedenharn and Gamba (1972) is applicable to symmetry groups, the Clebsch–Gordan coefficients of which are not explicitly known.

Although it was shown by Biedenharn and Gamba (1972) that the method works in some explicit examples a general proof of the rules of the method was lacking.

In this paper we shall present a different presentation of the techniques developed by Biedenharn and Gamba (1972), which proves the rules and clarifies the method in terms of the familiar concepts of the Racah–Wigner calculus§.

2. The physical problem

Let H_0 be the hamiltonian of a physical system and let $\mathscr{G}$ be the symmetry group of this system. We assume that we know precisely the spectrum of H_0, ie its eigenvectors

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§ Another paper which has the same in view is L Basano and R Cenni *Atomic Level Splitting by External Fields* (Genova preprint).

and corresponding eigenvalues. The eigenvectors can be labelled by the set of quantum numbers (J, M), where (J) denotes an irreducible representation of dimension $[J]$ of $\mathscr{G}$, whereas M specifies the $[J]$ basis vectors of the carrier space or representation space of (J). The eigenvalues depend only on J and we write them as a^J.

Now we introduce a perturbation hamiltonian H_1, with symmetry group $\mathscr{H}$ which is a subgroup of $\mathscr{G}$. The symmetry group of the total hamiltonian $H = H_0 + H_1$ is then also $\mathscr{H}$. The eigenvectors of $H = H_0 + H_1$ will be labelled by quantum numbers (j, m), where (j) is an irreducible representation of $\mathscr{H}$ and m denotes the basis vectors spanning the representation space of (j). In general the degenerate level corresponding to an irreducible representation (J) of $\mathscr{G}$ will split into levels corresponding to irreducible representations (j) of $\mathscr{H}$. The problem is now to determine the relative magnitudes of the shifts.

To specify the problem we assume that H_1 transforms under $\mathscr{G}$ as a component T_M^{K,τ_K} of an irreducible tensor operator T^{K,τ_K} of rank K or more generally as a linear combination

$$H_1 = \sum_M c_M T_M^{K,\tau_K} \equiv V_{K,\tau_K} \tag{1}$$

of such components. The index τ_K is a multiplicity index (cf § 5). The constants c_M have to be chosen in such a way that V_{K,τ_K} is an invariant of the subgroup $\mathscr{H}$ of $\mathscr{G}$ (cf § 3).

We want to know how the $[J]$ fold degenerate energy level corresponding to the irreducible representation (J) of $\mathscr{G}$ splits under the action of V_{K,τ_K}. From perturbation theory it is known that to this end one has to diagonalize the matrix with elements

$$\langle JM_1 | V_{K,\tau_K} | JM_2 \rangle, \tag{2}$$

the eigenvalues of which determine the energy shifts with respect to the unperturbed energy level. (In order to obtain real shifts we assume V_{K,τ_K} to be hermitian.)

Therefore we have to do with the eigenvalue problem of V_{K,τ_K} restricted to the representation space of (J). We shall denote this restriction of V_{K,τ_K} by $V_{K,\tau_K}(J)$.

As an example let us consider the splitting of an atomic level (characterized by the angular momentum L under the rotation group R_3) when placed in a crystalline field of octahedral symmetry (Biedenharn and Gamba 1972). We consider the quantitative effects of a symmetry-breaking hamiltonian, invariant under the octahedral group and transforming as a tensor operator V_K under R_3 (see equation (1)). The multiplicity index τ_K can be omitted in this case. By working out explicitly the perturbation equations (see Judd 1963 for details), one can write the results as in table 1.

The columns are labelled by (j_i) $(i = 1, 2, \ldots, 5)$ denoting the irreducible representations of the octahedral group. The rows labelled $V_K(0)$, $V_K(1)$, $V_K(2)$, etc give the quantitative splitting for the corresponding field. For example, from table 1 one can read off immediately that the energies of the three levels resulting from an $L = 3$ state are given by

$$E_1 = a - b + 9c \qquad \text{corresponding to } (j_2),$$

$$E_2 = a + 3b - 5c \qquad \text{corresponding to } (j_4),$$

$$E_3 = a - 6b - 12c \qquad \text{corresponding to } (j_5),$$

where a, b, c are the strengths of the perturbing fields transforming as V_0, V_4 and V_6 respectively.

It is clear that the entries in table 1 are the eigenvalues of the various operators $V_K(L)$ up to an L-dependent constant. The operator $V_4(2)$, for example, has a three-fold

Table 1.

L		j_1	j_2	j_3	j_4	j_5
0	$V_0(0)$	1	0	0	0	0
1	$V_0(1)$	0	0	0	1	0
2	$V_0(2)$	0	1	1	0	0
	$V_4(2)$	0	-2	3	0	0
3	$V_0(3)$	0	1	0	1	1
	$V_4(3)$	0	-1	0	3	-6
	$V_6(3)$	0	9	0	-5	-12
4	$V_0(4)$	1	1	1	1	0
	$V_4(4)$	14	-13	2	7	0
	$V_6(4)$	-20	-5	16	1	0
	$V_8(4)$	-10	0	-7	8	0
..	....	..	..	..	..	..

degenerate eigenvalue -2 and a doubly degenerate eigenvalue 3 up to a common factor (note that $[j_2] = 3$ and $[j_3] = 2$).

To avoid the elaborate and tedious diagonalization process to determine these eigenvalues Biedenharn and Gamba proposed a procedure, which is faster and rather elegant. Their method makes use of a set of heuristic rules which, for the convenience of the reader, will be given below (in our notation).

Biedenharn and Gamba consider the algebra generated by the irreducible representations (j_i), $i = 1, 2, \ldots, 5$, with multiplication rule

$$(j_1)\otimes(j_2) = \sum_{j_3} \{j_1 j_2 j_3\}(j_3),$$

where $\{j_1 j_2 j_3\}$ is a $3j$ symbol which gives the number of times that (j_3) is contained in $(j_1)\otimes(j_2)$. In this algebra they define elements

$$\hat{V}_K(L) = \sum_j a_j^{KL}(j),$$

which correspond to the above mentioned operators $V_K(L)$ and where the a_j^{KL} are the entires of the row labelled by $V_K(L)$ in table 1 (the ^ sign indicates that we now have to deal with elements of the representation algebra). Furthermore two kinds of products are defined for the $\hat{V}_K(L)$: the inner product

$$\hat{V}_K(L)\hat{V}_{K'}(L) = \sum_j a_j^{KL} a_j^{K'L}(j) \qquad [12]$$

and the outer product

$$\hat{V}_K(L)\otimes \hat{V}_{K'}(L') = \sum_{j_1 j_2 j_3} a_{j_1}^{KL} a_{j_2}^{K'L'} \{j_1 j_2 j_3\}(j_3). \qquad [13]$$

(The numbers between square brackets refer to the equations in Biedenharn and Gamba 1972.)

Next the trace of $\hat{V}_K(L)$ is defined to be

$$\mathrm{Tr}(\hat{V}_K(L)) = \sum_j a_j^{KL}[j]. \qquad [14]$$

The rules proposed by Biedenharn and Gamba are now:

$$\mathrm{Tr}\ \hat{V}_K(L) = [L]\delta_{K,0}, \qquad [15]$$

$$\mathrm{Tr}(\hat{V}_K(L)\hat{V}_{K'}(L)) = 0, \qquad K \neq K', \qquad [16]$$

$$\hat{V}_0(L) \otimes \hat{V}_K(L') = \text{linear combination of } \hat{V}_K(L''),$$

where

$$L'' = |L-L'|, |L-L'|+1, \ldots, L+L', \qquad [19]$$

and

$$\hat{V}_K(L)\hat{V}_{K'}(L) = \text{linear combination of } \hat{V}_{K''}(L)$$

with

$$K'' = |K-K'|, |K-K'|+1, \ldots, K+K'. \qquad [24]$$

These rules are sufficient to determine the entries of table 1, as soon as one knows the qualitative part of the splitting, ie which entries in the rows $V_0(L)$ are equal to one (this tells us which levels will play a role in the splitting). The orthogonality relation [16] provides us then immediately with the entries of the row $V_4(2)$. The entries of the row $V_4(3)$ can be determined by applying equation [19]. To this end one has to write $\hat{V}_4(3) = \alpha(j_2)+\beta(j_4)+\gamma(j_5)$ and to solve α, β and γ together with the constants A, B and C from the equation

$$\hat{V}_4(2) \otimes \hat{V}_0(1) = A\hat{V}_4(1)+B\hat{V}_4(2)+C\hat{V}_4(3)$$

(note that the coefficients α, β and γ are only defined up to a factor, which can be absorbed into C). The entries in the row $V_6(3)$ can immediately be found by using orthogonality with $V_0(3)$ and $V_4(3)$. With the same procedure one can complete the table for $L = 4$.

In the next sections we shall prove that the rules, applied above in the special case of the rotation group and one of its subgroups, hold for a large class of groups and subgroups and we shall point out to what extent the Biedenharn–Gamba method can be applied. This will be done by using the well known Racah–Wigner calculus for an arbitrary group and some character theory.

3. Inner and outer products

We shall introduce 'inner' and 'outer' products for the operators $V_{K,\tau_K}(J)$. To begin with we shall show that the coefficients c_M of equation (1) have to satisfy

$$\sum_{M'} D^{(K)}_{MM'}(R)c_{M'} = c_M, \qquad \forall\ R \in \mathscr{H}. \qquad (3)$$

The proof is very easy:

$$\begin{aligned} U_R V_{K,\tau_K} U_R^{-1} &= \sum_M c_M U_R T_M^{K,\tau_K} U_R^{-1} \\ &= \sum_M c_M \sum_{M'} D^{(K)}_{M'M}(R) T_{M'}^{K,\tau_K} \\ &= \sum_{M'} c_{M'} T_{M'}^{K,\tau_K} = V_{K,\tau_K}. \end{aligned} \tag{4}$$

(The U_R is a unitary operator representing the group element R in the same Hilbert space as in which V_{K,τ_K} operates, cf Edmonds 1957, Rose 1957 and Lomont 1959.) Equation (3) says that the vector $c = (c_1, c_2, \ldots, c_{[K]})$ is a simultaneous eigenvector of the set of matrices $D^{(K)}(R)$ with simultaneous eigenvalue 1, for all $R \in \mathscr{H}$.

Now the set of matrices $D^{(K)}(R)$, $R \in \mathscr{H}$, form a representation of $\mathscr{H}$ (which is in general reducible). So we can also formulate the above statement by saying that the one-dimensional subspace spanned by the vector c is the representation space of the trivial representation (1_1) of $\mathscr{H}$. From this it follows that one can find a vector c satisfying equation (3) if and only if the irreducible representation (K) of $\mathscr{G}$, restricted to $\mathscr{H}$ contains the trivial representation (1_1) of $\mathscr{H}$ at least once. More specifically, if this restriction contains the trivial representation (1_1) of $\mathscr{H}$ n times, then one can find n linearly independent vectors c, satisfying equation (3) and therefore also n linearly independent operators V_{K,τ_K} can be constructed out of a certain set $T_M^{K,\tau_K}(M = 1, \ldots, [K])$.

In order to introduce 'inner' and 'outer' products of operators of the type $V_{K,\tau_K}(J)$, we first limit ourselves to the operators $T_M^{K,\tau_K}(J)$ and $S_{M'}^{K',\tau_{K'}}(J')$ (ie the restrictions of T_M^{K,τ_K} and $S_{M'}^{K',\tau_{K'}}$ to the representation spaces of (J) and (J') respectively).

According to a well known principle (Edmonds 1957, Rose 1957) one can construct new irreducible tensor operators $U_{M''}^{K'',\tau_{K''}}$ from T_M^{K,τ_K} and $S_{M'}^{K',\tau_{K'}}$:

$$U_{M''}^{K'',\tau_{K''}} = [K'']^{1/2} \begin{pmatrix} \tau_{K''} & M'' & K & K' \\ & K'' & M & M' \end{pmatrix}^* T_M^{K,\tau_K} * S_{M'}^{K',\tau_{K'}} \tag{5}$$

(here the convention for summation over repeated indices is assumed). In (5) the symbol $(\ldots)$ is a $3jm$ symbol of Clebsch–Gordan coefficient, in which the multiplicity parameter $\tau_{K''}$ numbers the several irreducible representations (K'') which are contained in $(K)\otimes(K')$. The asterisk in $T_M^{K,\tau_K} * S_{M'}^{K',\tau_{K'}}$ stands for ordinary operator multiplication if T_M^{K,τ_K} and $S_{M'}^{K',\tau_{K'}}$ operate in the same Hilbert space. If T_M^{K,τ_K} and $S_{M'}^{K',\tau_{K'}}$ operate in different Hilbert spaces it means a direct product. In both cases the $U_{M''}^{K'',\tau_{K''}}$ are the components of an irreducible tensor operator of rank K'' (cf Edmonds 1957, Rose 1957).

From equation (5) it follows that

$$T_M^{K,\tau_K} * S_{M'}^{K',\tau_{K'}} = \sum_{K'',\tau_{K''}} [K'']^{1/2} \begin{pmatrix} \tau_{K''} & M'' & K & K' \\ & K'' & M & M' \end{pmatrix} U_{M''}^{K'',\tau_{K''}}. \tag{6}$$

First we consider the case that T_M^{K,τ_K} and $S_{M'}^{K',\tau_{K'}}$ operate in the same Hilbert space. We restrict all operators of equation (6) to the same subspace (J), which provides us with

$$T_M^{K,\tau_K}(J) S_{M'}^{K',\tau_{K'}}(J) = \sum_{K'',\tau_{K''}} [K'']^{1/2} \begin{pmatrix} \tau_{K''} & M'' & K & K' \\ & K'' & M & M' \end{pmatrix} U_{M''}^{K'',\tau_{K''}}(J). \tag{7}$$

We shall call this expression the inner product of $T_M^{K,\tau_K}(J)$ and $S_{M'}^{K',\tau_{K'}}(J)$. Next we suppose T_M^{K,τ_K} and $S_{M'}^{K',\tau_{K'}}$ to be operators in different Hilbert spaces and restrict them to subspaces (J) and (J') respectively. We define the outer product of $T_M^{K,\tau_K}(J)$ and $S_{M'}^{K',\tau_{K'}}(J')$ as

$$T_M^{K,\tau_K}(J)\otimes S_{M'}^{K',\tau_{K'}}(J') = \sum_{K'',\tau_{K''}} [K'']^{1/2}\begin{pmatrix}\tau_{K''} & M'' & K & K' \\ & K'' & M & M'\end{pmatrix} U_{M''}^{K'',\tau_{K''}}(J\otimes J'). \tag{8}$$

Now we consider the operators

$$V_{K,\tau_K}(J) = \sum_M c_M T_M^{K,\tau_K}(J) \qquad \text{and} \qquad V_{K',\tau_{K'}}(J) = \sum_{M'} d_{M'} T_{M'}^{K',\tau_{K'}}(J),$$

where the vector c satisfies equation (2) and the vector d satisfies

$$\sum_{M'} D_{MM'}^{(K')}(R)\, d_{M'} = d_M, \qquad \forall\, R\in\mathscr{H}. \tag{9}$$

From equation (7) we have

$$\begin{aligned} V_{K,\tau_K}(J)V_{K',\tau_{K'}}(J) &= \sum_{M,M'} c_M d_{M'} T_M^{K,\tau_K}(J) S_{M'}^{K',\tau_{K'}}(J) \\ &= \sum_{K'',\tau_{K''}}\sum_{M,M',M''} [K'']^{1/2}\begin{pmatrix}\tau_{K''} & M'' & K & K' \\ & K'' & M & M'\end{pmatrix} c_M d_{M'} U_{M''}^{K'',\tau_{K''}}(J) \\ &= \sum_{K'',\tau_{K''}}\sum_{M''} f_{M''} U_{M''}^{K'',\tau_{K''}}(J). \end{aligned} \tag{10}$$

The vector f (we suppressed the K, K', K'' and $\tau_{K''}$ dependence) with components $f_{M''}$ $(M'' = 1, 2, \ldots, [K''])$ has again the property

$$\sum_{M''} D_{N''M''}^{(K'')}(R) f_{M''} = f_{N''}, \qquad \forall\, R\in\mathscr{H}. \tag{11}$$

The proof is as follows:

$$\begin{aligned} \sum_{M''} D_{N''M''}^{(K'')}(R) f_{M''} &= \sum_{M,M',M''} [K'']^{1/2} D_{N''M''}^{(K'')}(R)\begin{pmatrix}\tau_{K''} & M'' & K & K' \\ & K'' & M & M'\end{pmatrix} c_M d_{M'} \\ &= \sum_{M,M'}\sum_{N,N'} [K'']^{1/2}\begin{pmatrix}\tau_{K''} & N'' & K & K' \\ & K'' & N & N'\end{pmatrix} D_{NM}^{(K)}(R) D_{N'M'}^{(K')}(R) c_M d_{M'} \\ &= \sum_{N,N'} [K'']^{1/2}\begin{pmatrix}\tau_{K''} & N'' & K & K' \\ & K'' & N & N'\end{pmatrix} c_N d_{N'} = f_{N''}, \qquad \forall\, R\in\mathscr{H}. \end{aligned}$$

We applied equations (3), (9) and equation (5-145) of Hamermesh (1964) adapted in such a way as to include a multiplicity index (cf also Wigner 1965).

This result allows us to write equation (10) as

$$V_{K,\tau_K}(J)V_{K',\tau_{K'}}(J) = \sum_{K'',\tau_{K''}} A_{K'',\tau_{K''}} V_{K'',\tau_{K''}}(J) \tag{12}$$

in which the $A_{K'',\tau_{K''}}$ are certain numerical constants. The coefficients $A_{K'',\tau_{K''}}$ vanish if the $3j$ symbol $\{K\ K'\ K''\} = 0$. The multiplicity index $\tau_{K''}$ numbers the different ways in which (K'') is contained in $(K)\otimes(K')$.

Along the same lines we can derive

$$V_{K,\tau_K}(J)\otimes V_{K',\tau_{K'}}(J') = \sum_{K'',\tau_{K''}} B_{K'',\tau_{K''}} V_{K'',\tau_{K''}}(J\otimes J') = \sum_{K'',\tau_{K''}} \sum_{J'',\tau_{J''}} C^{J'',\tau_{J''}}_{K'',\tau_{K''}} V_{K'',\tau_{K''}}(J'',\tau_{J''}), \tag{13}$$

where the $B_{K'',\tau_{K''}}$ and the $C^{J'',\tau_{J''}}_{K'',\tau_{K''}}$ are again certain numerical constants. The constants $C^{J'',\tau_{J''}}_{K'',\tau_{K''}}$ vanish if $\{K\ K'\ K''\} = 0$ or $\{J\ J'\ J''\} = 0$.

To show the relationship with the 'inner' and 'outer' products defined by Biedenharn and Gamba (1972) we shall write the operators $V_{K,\tau_K}(J)$ in an alternative way. Let

$$(J) = \sum_{j,\rho_j}^{\oplus} (j)_{\rho_j} \tag{14}$$

be the reduction of the irreducible representation (J) of $\mathscr{G}$ to irreducible representation (j) of $\mathscr{H}$ (ρ_j is a multiplicity index). We shall denote the orthonormal basis vectors of the representation space of (j) by $|jm;\rho_j\rangle$ ($m = 1, 2, \ldots, [j]$). We know that these vectors are eigenvectors of $V_{K,\tau_K}(J)$ and that the eigenvalues $a^{K\tau_K J}_{j\rho_j}$ do not depend on m, because of the invariance of $V_{K,\tau_K}(J)$ with respect to $\mathscr{H}$. Therefore we can write

$$V_{K,\tau_K}(J) = \sum_{j,\rho_j,m} |jm;\rho_j\rangle a^{K\tau_K J}_{j\rho_j} \langle jm;\rho_j|, \tag{15}$$

in which the same j occur as in equation (14).

In general two operators $V_K(J)$ and $V_{K'}(J)$ cannot be brought in diagonal form simultaneously. One has

$$\langle j_1 m_1 \rho_1 | V_K(J) | j_2 m_2 \rho_2 \rangle = A(j_1\rho_1\rho_2)\delta_{j_1 j_2}\delta_{m_1 m_2} \tag{16}$$

and

$$\langle j_1 m_1 \rho_1 | V_{K'}(J) | j_2 m_2 \rho_2 \rangle = A'(j_1\rho_1\rho_2)\delta_{j_1 j_2}\delta_{m_1 m_2}. \tag{17}$$

We have applied here the Wigner–Eckart theorem, noting that $V_K(J)$ is an invariant of the group $\mathscr{H}$. By performing a unitary transformation one can always bring $A(j_1\rho_1\rho_2)$ into a form $A(j_1\rho_1)\delta_{\rho_1\rho_2}$. However, in general then $A'(j_1\rho_1\rho_2)$ will not simultaneously be in the form $A'(j_1\rho_1)\delta_{\rho_1\rho_2}$. From this discussion it is clear that if the restrictions of the representations (K) and (K') of $\mathscr{G}$ to irreducible representations (j) of $\mathscr{H}$ are multiplicity free, then $V_K(J)$ and $V_{K'}(J)$ can be brought to diagonal form simultaneously. From now on we shall consider cases in which these restrictions are multiplicity free. For the inner product of $V_{K,\tau_K}(J)$ and $V_{K',\tau_{K'}}(J)$ we then have immediately

$$\begin{aligned} V_{K,\tau_K}(J)V_{K',\tau_{K'}}(J) &= \sum_{j,\rho_j,m} \sum_{j',\rho_{j'},m'} |jm;\rho_j\rangle a^{K\tau_K J}_{j\rho_j} \langle jm;\rho_j | j'm';\rho_{j'}\rangle a^{K'\tau_{K'} J}_{j'\rho_{j'}} \langle j'm';\rho_{j'}| \\ &= \sum_{j,\rho_j,m} |jm;\rho_j\rangle a^{K\tau_K J}_{j\rho_j} a^{K'\tau_{K'} J}_{j\rho_j} \langle jm;\rho_j|. \end{aligned} \tag{18}$$

In the same way we have for the outer product in the multiplicity-free case

$$V_{K,\tau_K}(J)\otimes V_{K',\tau_{K'}}(J) = \sum_{j,\rho_j,m} \sum_{j',\rho_{j'},m'} |jm;\rho_j\rangle \otimes |j'm';\rho_{j'}\rangle a^{K\tau_K J}_{j\rho_j} a^{K'\tau_{K'} J'}_{j'\rho_{j'}} \langle jm;\rho_j| \otimes \langle j'm';\rho_{j'}|. \tag{19}$$

If one defines

$$|j''m'';\sigma_{j''}\rho_j\rho_{j'}\rangle = \sum_{m,m'} [j'']^{1/2} \begin{pmatrix} \sigma_{j''} & m'' & j & j' \\ & j'' & m & m' \end{pmatrix}^* |jm;\rho_j\rangle \otimes |j'm';\rho_{j'}\rangle \quad (20)$$

one can derive with the help of an orthogonality relation for $3jm$ symbols that

$$V_{K,\tau_K}(J) \otimes V_{K',\tau_{K'}}(J') = \sum_{jj'j''m''} \sum_{\rho_j\rho_{j'}\sigma_{j''}} |j''m'';\sigma_{j''}\rho_j\rho_{j'}\rangle a_{j\rho_j}^{K\tau_K J'} a_{j'\rho_{j'}}^{K'\tau_{K'}J'} \langle j''m'';\sigma_{j''}\rho_j\rho_{j'}|. \quad (21)$$

Equations (18) and (21) are a more general and more precise form of equations [12] and [13] of Biedenharn and Gamba (1972). Now we have verified that the definitions in this paper of inner and outer product are equivalent to those of Biedenharn and Gamba (1972) in the multiplicity-free case and therefore it follows immediately that equations (12) and (13) of this paper prove the heuristic rules of equations [24] and [19] of Biedenharn and Gamba (1972) and are even a generalization of these rules (note the $\tau_{J''}$ and the $\tau_{K''}$ in equation (13)). Our discussion also makes clear why the definitions [12] and [13] of Biedenharn and Gamba (1972) cannot be maintained in the non-multiplicity-free case.

4. The trace operation

We define the trace of the operator $V_{K,\tau_K}(J)$ in the conventional way, as being the sum of its diagonal elements in some matrix representation. By means of equation (15) it can immediately be seen that the definition in Biedenharn and Gamba (1972) (see equation [14] of Biedenharn and Gama 1972) is equivalent to ours:

$$\begin{aligned} \operatorname{Tr} V_{K,\tau_K}(J) &= \sum_{j',\rho_{j'},m'} \sum_{j,\rho_j,m} \langle j'm';\rho_{j'}|jm;\rho_j\rangle a_{j\rho_j}^{K\tau_K J} \langle jm;\rho_j|j'm';\rho_{j'}\rangle \\ &= \sum_{j,\rho_j,m} a_{j\rho_j}^{K\tau_K J} = \sum_{j,\rho_j} [j] a_{j\rho_j}^{K\tau_K J}. \end{aligned} \quad (22)$$

We can also prove the heuristic rules concerning this trace operator, given in equations [15] and [16] of Biedenharn and Gamba (1972). Equation [15] of Biedenharn and Gamba (1972) can be proved very easily:

$$\begin{aligned} \operatorname{Tr} V_{K,\tau_K}(J) &= \sum_{M,M_1} c_M \langle JM_1|T_M^{K,\tau_K}|JM_1\rangle \\ &= \sum_{M,M_1} c_M \begin{pmatrix} \tau_K & M_1 & K & J \\ & J & M & M_1 \end{pmatrix} \langle J\|T^{K,\tau_K}\|J\rangle \\ &= c_1 \langle J\|T^{(1_1)}\|J\rangle \delta_{K,(1_1)}. \end{aligned} \quad (23)$$

In equation (23) $\langle J\|T^{K,\tau_K}\|J\rangle$ denotes a reduced matrix element. In the derivation of the above equation a generalization of equation (15) of Wigner (1965) has been used (cf also Hamermesh 1964). We remark that in principle the same proof has been given in the examples in § 3 of Biedenharn and Gamba (1972).

Furthermore we have

$$\operatorname{Tr}(V_{K,\tau_K}(J) V_{K',\tau_{K'}}(J)) = \sum_{K'',\tau_{K''}} A_{K'',\tau_{K''}} \operatorname{Tr} V_{K'',\tau_{K''}}(J) = A_{(1_1)} \delta_{K^*,K'} \operatorname{Tr} V_{(1_1)}(J). \quad (24)$$

((K^*) is the complex conjugate representation of (K)). In particular

$$\mathrm{Tr}(V_{K,\tau_K}(J)V_{K',\tau_{K'}}(J)) = 0, \qquad \text{if } K^* \neq K'. \tag{25}$$

We remark that if $K^* = K'$ it is always possible to orthogonalize the set $V_{K,\tau_K}(J)$, where τ_K varies over the multiplicity index set of a fixed K, such that

$$\mathrm{Tr}(V_{K,\tau_K}(J)V_{K^*,\bar{\tau}_K}(J)) = 0, \qquad \text{if } \tau_K \neq \bar{\tau}_K. \tag{26}$$

It can easily be proved that the normalization

$$\mathrm{Tr}\,(V_{K,\tau_K}(J)V_{K,\tau_K}(J)) = [K]^{-1}$$

corresponds with $\Sigma_M\,|c_M^2| = 1$ and $|\langle J\|T^{K,\tau_K}\|J\rangle| = 1$.

5. Discussion of the multiplicity problem

In the previous sections we have met multiplicities of various kinds:

(i) a multiplicity (denoted by σ) originating from the fact that the reduction of Kronecker products of two irreducible representations of $\mathscr{H}$ is not multiplicity-free in general;

(ii) a multiplicity (denoted by τ) originating from the fact that the reduction of Kronecker products of two irreducible representations of $\mathscr{G}$ is not multiplicity-free in general;

(iii) a multiplicity (denoted by ρ) originating from the fact that the restriction of an irreducible representation of $\mathscr{G}$ to irreducible representations of $\mathscr{H}$ is not multiplicity-free in general.

There is a fourth multiplicity which has to do with the independent ways in which one can construct vectors c satisfying equation (3). However, as was discussed in § 3 one can find n linearly independent vectors c if and only if the restriction of the irreducible representation (K) of $\mathscr{G}$ contains the trivial representation (1_1) of $\mathscr{H}$ n times. Therefore this multiplicity is a special case of (iii). The multiplicity described under (i) does not give any troubles, because the $V_{K,\tau_K}(J)$ do not depend on them. The multiplicity described under (ii) is also not very serious. In this case it is possible that the index τ_K in $V_{K,\tau_K}(J)$ varies over a range of values. The amounts of splitting cannot be determined then by applying the rules proposed (for the multiplicity-free case) by Biedenharn and Gamba, because in general one does not have means to distinguish between $V_{K,\tau_K}(J)$-operators for different values of τ_K. If one has means to distinguish between such operators (as in SU(3) where one has a symmetric and an antisymmetric octet operator) then one finds unambiguous answers.

The multiplicity mentioned under (iii) is much more serious. As was discussed in § 3 two operators $V_{K,\tau_K}(J)$ and $V_{K',\tau_{K'}}(J)$ can in general not be brought simultaneously into diagonal form, in the non-multiplicity-free case. This implies that the definitions of the inner and outer products of equations [12] and [13] of Biedenharn and Gamba (1972) cannot be maintained and therefore the procedure of Biedenharn and Gamba (1972) breaks down. If $V_{K,\tau_K}(J)$ and $V_{K',\tau_{K'}}(J)$ cannot be diagonalized simultaneously the orthogonality relation (24) remains valid, but we cannot use equation (18) to calculate the inner product.

We shall now comment on a related aspect of the multiplicity problem. If one considers table 1 of this paper (giving the quantitative splitting of levels with angular momentum $L = 1, 2, 3, 4, \ldots$ in a field of octahedral symmetry) one observes that for fixed L the number of participating $V_K(L)$ operators equals the number of irreducible representations (j_k) of the octahedral group, which play a role in splitting the level (L). One can prove that this is true in general, as soon as the restriction of the irreducible representation (J) of $\mathscr{G}$ to irreducible representations (j) of the subgroup $\mathscr{H}$ is multiplicity-free.

Proof. Let (J) be a fixed irreducible representation of $\mathscr{G}$ and let its reduction to irreducible representations (j) of $\mathscr{H}$ be multiplicity-free. We saw in the previous sections that if $V_K(J)$ is to be an invariant non-vanishing operator with respect to $\mathscr{H}$, the following requirements have to be fulfilled:

$$\{J \quad K \quad J\} = \{J \quad J^* \quad K\} > 0 \tag{27}$$

and

$$\frac{1}{h}\sum_{S\in\mathscr{H}} \chi^{(K)}(S) > 0, \tag{28}$$

where $\chi^{(K)}(S)$ is the character of the group element S in the representation (K).

This last equation expresses the fact that the irreducible representation (K) restricted to $\mathscr{H}$ contains (1_1) of $\mathscr{H}$ at least once. More precisely the total number of irreducible representations (K) which fulfil equations (27) and (28) is given by

$$\begin{aligned} n(J) &= \sum_K \{J \quad J^* \quad K\}\frac{1}{h}\sum_{S\in\mathscr{H}} \chi^{(K)}(S) \\ &= \frac{1}{hg}\sum_K \sum_{S\in\mathscr{H}} \sum_{R\in\mathscr{G}} \chi^{(J)}(R)\chi^{(J)*}(R)\chi^{(K)*}(R)\chi^{(K)}(S) \\ &= \frac{1}{h}\sum_{S\in\mathscr{H}} \sum_{R\in\mathscr{G}} |\chi^{(J)}(R)|^2 \frac{1}{g_R}\delta(\mathscr{C}_S, \mathscr{C}_R). \end{aligned} \tag{29}$$

The δ symbol in the right-hand side of this equation is equal to 1 if the classes $\mathscr{C}_S$ and $\mathscr{C}_R$ of $\mathscr{G}$ in which the elements S and R lie respectively are the same, and is equal to 0 otherwise. The number g_R is the number of elements of $\mathscr{G}$ lying in $\mathscr{C}_R$. We can perform the summation over S giving

$$n(J) = \frac{1}{h}\sum_{R\in\mathscr{G}} |\chi^{(J)}(R)|^2 \frac{h_R}{g_R} = \frac{1}{h}\sum_{R\in\mathscr{H}} |\chi^{(J)}(R)|^2. \tag{30}$$

In this equation h_R stands for the number of elements of $\mathscr{H}$ lying in $\mathscr{C}_R$.

If

$$(J) = \sum_{j,\rho_j}^{\oplus} (j)_{\rho_j} = \sum_j^{\oplus} b_j^J(j), \tag{31}$$

where b_j^J denotes the number of times that a certain irreducible representation (j) occurs in the restriction of (J) to $\mathscr{H}$, it follows that

$$\chi^{(J)}(R) = \sum_j b_j^J \chi^{(j)}(R), \qquad R \in \mathscr{H}. \tag{32}$$

Therefore we can write

$$n(J) = \sum_j (b_j^J)^2. \tag{33}$$

In the case that the restriction of (J) to $\mathscr{H}$ is multiplicity-free, the numbers b_j^J are equal to 1 or 0 and thus

$$n(J) = \sum_j b_j^J. \tag{34}$$

The right-hand side of equation (34) just equals the number of irreducible representations of $\mathscr{H}$, which are contained in (J)‡.

From the above proof it also follows that in the non-multiplicity-free case one has

$$n(J) > \sum_j b_j^J, \tag{35}$$

ie the number of rows in schemes like table 1 is larger than the number of columns. This shows once more that for fixed J not all the 'row vectors' in such a scheme can be orthogonal to each other in the sense that

$$\sum_{j,\rho_j} a_{j\rho_j}^{K,\tau_K J}[j] = 0$$

if $(K, \tau_K) \neq (K', \tau_{K'})$.

Acknowledgments

We thank Professor Biedenharn for suggesting this problem to us and for providing some unpublished notes of Professor Gamba on this problem.

One of us (AJvZ) would like to thank the Netherlands America Commission for Educational Exchange for financial support. This research was supported in part by the National Science Foundation and the Army Research Office (Durham).

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‡ One can give a slightly different proof which is also valid in the case of compact continuous groups. We are indebted to Dr R King of the University of Southampton for his remark regarding this point.