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Commuting tensor operators and the state labelling problem for SO(4) ⊃ P

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Abstract. The application of irreducible tensor techniques to state labelling problems is described. For the pentahedral subgroup of SO(4) it is demonstrated that a solution to the labelling problem using a set of mutually commuting operators is not possible if we demand that each of the operators transform irreducibly under SO(4).

1. Introduction

If one is contemplating using a set of mutually commuting operators to resolve the state labelling problem, it is of some importance to know how many operators are required in the set and indeed even whether a suitable commuting set exists. To this end we have investigated the labelling problem for SO(4) ⊃ P where P is the pentahedral subgroup of SO(4). We have found that a solution in terms of a set of commuting operators each symmetrised with respect to an irreducible representation (irrep) of SO(4) is not possible.

In obtaining our results we have made extensive use of group tensor operators and Kronecker product theory. While these techniques are quite standard, their application to the state labelling problem is somewhat novel. We therefore think it appropriate to briefly discuss the relationship between labelling operators and group tensors and to present a few simple results (including striking symmetries among the eigenvalues) which highlight the insight which such an approach gives. Armed with these general results we are then able to proceed to discuss the specific case SO(4) ⊃ P, transforming to a canonical basis for actual calculations.

At the outset we restrict our labelling considerations to what may be termed physically appropriate bases for the Hilbert space, i.e. those which display the symmetry of the relevant Hamiltonian. Thus if a hierarchy of groups $G \supset H$ is evident, then using Dirac's bra–ket notation we wish to write the basis states as the kets $|\Gamma\, a\, \gamma\, i\rangle$ where Γ is an irrep of G, γ an irrep of H, i an extra label needed if γ is greater than one-dimensional and a another additional label required in case of branching multiplicity in the reduction of Γ to γ under restriction of the operations of G to those of H.

The irrep labels Γ and γ are normally fairly easy to assign and for the label i we can use further subgroups to provide labels if necessary. However, the resolution of the branching multiplicity label a is usually a more difficult task. Our aim will be to resolve it by using the eigenvalues of a set of mutually commuting operators. We emphasise that we are concerned only with operators which resolve the branching multiplicity and not necessarily with operators which completely distinguish every partner of Γ.

Suppose that G is a Lie group, then if the labelling operators are constructed from the generators of G they will commute with the Casimir invariants of G (which of course may be used to label Γ) and also with the physical Hamiltonian. Such operators might be the symmetric polynomials which are homogeneous of degree n in the generators. (We shall see later that the homogeneous condition is an undesirable restriction.) These operators belong to the universal enveloping algebra, U of the Lie algebra of G. In order for them to be capable of resolving the branching multiplicity it is necessary (and we shall see soon why) that they be invariant under H.

The enumeration of these invariants is closely related to Hilbert's fourteenth problem. Briefly, this poses the question: 'If G acts linearly on the variables $x_1, \ldots, x_r$, are the H-invariant polynomials in these variables finitely generated?' The answer in general is negative (Nagata 1958) but if H is a finite or compact group then the answer is in the affirmative. A set of invariants from which all others can be constructed is termed an integrity basis (Weyl 1946). The concept of an integrity basis for invariant operators was examined by Judd *et al* (1974). They showed that there was a one-to-one correspondence between invariants in U and invariants in the space of polynomials in the variables $x_1, \ldots, x_r$. The integrity basis for operators, though, is in general smaller because of the commutation relations that exist among the generators.

Recent use of invariant operators to resolve labelling problems includes the work of Patera and Winternitz (1973, 1976) and Bickerstaff and Wybourne (1976) on the finite subgroups of SO(3), Judd *et al* (1974) on $SU(3) \supset SO(3)$ and Quesne (1976, 1977) on $SU(4) \supset SU(2) \times SU(2)$. Except for the latter, these rely on a single operator to resolve branching multiplicities. A rather vaguely stated theorem of Racah (1951) purportedly tells us when a single operator is inadequate for labelling purposes. Because of this theorem, $SO(4) \supset P$ has generally been thought to be a case of a 'two missing labels problem.' We shall see from our study of this example that Racah's theorem does have limited application.

As we have already mentioned, our approach uses group tensors. These are manipulated by the Wigner–Racah algebra which has been generalised for finite or compact groups by Derome and Sharp (1965), Derome (1966) and Butler (1975). Butler's work pays particular attention to phase problems and consistency of notation. The notation we shall use to describe the various aspects of the generalised Wigner–Racah algebra follows that suggested by Butler in his conclusion.

2. The labelling operators as group tensors

The homogeneous polynomials in the generators of G act linearly on the Hilbert space. Also they can be symmetrised so as to transform irreducibly under the actions of G. Accordingly they behave as group tensors (see Butler 1975). We shall write the symmetrised labelling operators as $T^{n}{}^{\alpha\Gamma}_{a0}$ where n is the degree of the polynomial, Γ is an irrep of G, a is a branching multiplicity label and 0 denotes the identity irrep of H (α is an extra label in case there is more than one invariant of degree n with the same transformation properties).

As is well known, the generators form a vector space over the field of complex numbers. Construction of homogeneous polynomials in these generators is closely related to forming tensor powers of this vector space. Further, the vector space will transform as a representation Γ_g of G. (Γ_g will usually be irreducible, but not always.) Thus the irreps of G under which the homogeneous polynomials of degree n may transform are those occurring in the nth Kronecker powers of Γ_g.

However, the operators in U are symmetric polynomials and therefore they can only transform according to representations which occur in the totally symmetric part of the Kronecker powers of Γ_g. The decomposition of the various symmetry parts of the Kronecker powers into irreps may be readily found using Littlewood's (1950) algebra of plethysm. Hence, the symmetric invariants transform according to the irreps occurring in $\Gamma_g \otimes \{n\}$. The plethysm may be evaluated using the methods described by Wybourne (1970a) and Butler and King (1973). (Butler and Wybourne (1971) have compiled a useful table of plethysms.) If there are r generators then the degree of this plethysm is $(n+r-1)!/n!(r-1)!$ which gives the total number of symmetric nth-order polynomials in the generators—a result familiar to classical invariant theory.

In order to enumerate the symmetric invariants we now need only know the branching rules for the restriction $G \to H$. There are many available methods for evaluating branching rules but several of the more common ones are tedious and we draw attention to the use of S-functions and the work of King (1975).

Before proceeding further we note that all of the compact Lie groups are quasi-ambivalent and Butler and King (1974), Butler (1975) and Butler and Wybourne (1976) have discussed various simplifying choices in the Wigner–Racah algebra which are possible for these groups. Since we shall only be considering compact Lie groups we shall assume these simplifications in what follows.

3. Properties of matrix elements

Any group tensor operator obeys the Wigner–Eckart theorem (Butler 1975) and this is true in particular of the labelling operators. Also, since the labelling operators are constructed from the generators of G they are diagonal in the irreps of G. Further simplifications in the Wigner–Eckart theorem occur because they are invariant under the subgroup H. Using the Racah factorisation lemma for the 2-jm and 3-jm symbols and the definition and orthogonality of the 2-jm symbols for H (and simplifications in the 2-jm factors noted by Butler and Wybourne 1976) we obtain

$$\begin{aligned}\langle \Gamma_1\, a_1\, \gamma_1\, i_1 | T^{n\,\alpha\Gamma}_{\;\;a0} | \Gamma_2\, a_2\, \gamma_2\, i_2\rangle &= |\gamma_1|^{-1/2} \sum_r \begin{pmatrix} \Gamma_1 & \Gamma_1^* \\ a_1\,\gamma_1 & a_1^*\,\gamma_1^* \end{pmatrix} \begin{pmatrix} \Gamma_1^* & \Gamma & \Gamma_2 \\ a_1^*\,\gamma_1^* & a0 & a_2\,\gamma_2 \end{pmatrix}^r \\ &\quad \times \langle \Gamma_1 \| \mathbf{T}^{n\alpha\Gamma} \| \Gamma_2\rangle_r\, \delta_{\Gamma_1\Gamma_2}\, \delta_{\gamma_1\gamma_2}\, \delta_{i_1 i_2} \end{aligned} \tag{1}$$

where * denotes the contragredient label and r is a Kronecker product multiplicity label. This expression, in terms of the 2-jm and 3-jm factors shows that the invariants are diagonal in the irrep labels of G and H and not only diagonal in any additional labels at a lower group level but also the values of the diagonal matrix elements are entirely independent of them. Thus the eigenvalues of an invariant operating on the Γ_1 module are degenerate with degeneracies at least equal to the dimensions of the irreps γ_1 of H which appear in the decomposition of Γ_1 under the restriction $G \to H$.

This agrees of course with what we expect from Schur's lemma and is the reason why we want to consider invariants as labelling operators.

If the eigenvalues are different for different branching multiplicity labels then the problem is solved. It is not obvious that this will be so, however. Indeed if the operator is of high enough degree in the generators then it is clear that such an operator could well have all zero eigenvalues for some modules because the Kronecker product condition $\Gamma_1^* \times \Gamma \times \Gamma_1 \supset 0$ might not be satisfied. Casimir invariants of H would also be unsuitable.

Let us examine the eigenvalue spectrum further.

The sum of the eigenvalues is given by the trace of the invariant. For the Γ_1 module we have

$$\mathrm{Tr}(T^{n\,\alpha\Gamma}_{\ \ a0}) = \sum_{a_1\gamma_1} |\gamma_1|^{+1/2} \sum_r \begin{pmatrix} \Gamma_1 & \Gamma_1^* \\ a_1\,\gamma_1 & a_1^*\,\gamma_1^* \end{pmatrix} \begin{pmatrix} \Gamma_1^* & \Gamma & \Gamma_1 \\ a_1^*\,\gamma_1^* & a0 & a_1\,\gamma_1 \end{pmatrix}^r \langle \Gamma_1 \| \mathbf{T}^{n\alpha\Gamma} \| \Gamma_1 \rangle_r. \tag{2}$$

From the orthogonality properties of the 3-*jm* factors and the definition of the 2-*jm* factor (remembering that it is chosen real) it is simple to deduce that

$$\sum_{a_1\gamma_1} |\gamma_1|^{+1/2} \begin{pmatrix} \Gamma_1 & \Gamma_1^* \\ a_1\,\gamma_1 & a_1^*\,\gamma_1^* \end{pmatrix} \begin{pmatrix} \Gamma_1^* & \Gamma & \Gamma_1 \\ a_1^*\,\gamma_1^* & a0 & a_1\,\gamma_1 \end{pmatrix}^r = |\Gamma_1|^{+1/2}\, \delta_{r0}\, \delta_{\Gamma 0}\, \delta_{a0}. \tag{3}$$

Changing the order of summation in equation (2) and using equation (3) we obtain the result that

$$\mathrm{Tr}(T^{n\,\alpha\Gamma}_{\ \ a0}) = \delta_{\Gamma 0} |\Gamma_1|^{+1/2} \langle \Gamma_1 \| \mathbf{T}^{n\alpha\Gamma} \| \Gamma_1 \rangle \tag{4}$$

which shows that the invariants are traceless unless they transform as the identity irrep of G. Indeed, exactly the same result can be shown to be true for any tensor operator (and not just invariants), as is well known. The proof is a trivial modification of the above, using the orthogonality properties of the 3-*jm* symbols rather than the 3-*jm* factors, and is a generalisation to all finite or compact groups of the proof of Fano and Racah (1959) for the angular momentum tensors.

What about the sum of the moduli of the eigenvalues? We deduce this from the trace of $(T^{n\,\alpha\Gamma}_{\ \ a0})^+ (T^{n\,\alpha\Gamma}_{\ \ a0})$. It is not difficult to show that

$$\mathrm{Tr}(T^{n\,\alpha\Gamma\,+}_{\ \ a0}\, T^{n\,\alpha\Gamma}_{\ \ a0}) = |\Gamma|^{-1} \sum_r |\langle \Gamma_1 \| \mathbf{T}^{n\alpha\Gamma} \| \Gamma_1 \rangle_r|^2 \tag{5}$$

and again this result holds for all tensors. It is clear that similar results could be found for higher degree products of the eigenvalues.

We come now to the implications of permutation symmetries of the 2-*jm* and 3-*jm* factors. Using these symmetries in equation (1) and the fact that the 2-*j* symbols are of norm unity we find that

$$\begin{aligned} &\langle \Gamma_1^*\, a_1^*\, \gamma_1^*\, i_1 | T^{n\,\alpha\Gamma}_{\ \ a0} | \Gamma_1^*\, a_1^*\, \gamma_1^* i_1 \rangle \\ &\quad = |\gamma_1|^{-1/2} \sum_{rt} \{\Gamma_1\, \Gamma_1^*\}\{(13), \Gamma_1^*\, \Gamma\, \Gamma_1\}_{rt} \begin{pmatrix} \Gamma_1 & \Gamma_1^* \\ a_1\,\gamma_1 & a_1^*\,\gamma_1^* \end{pmatrix} \\ &\quad\quad \times \begin{pmatrix} \Gamma_1^* & \Gamma & \Gamma_1 \\ a_1^*\,\gamma_1^* & a0 & a_1\,\gamma_1 \end{pmatrix}^t \langle \Gamma_1^* \| \mathbf{T}^{n\alpha\Gamma} \| \Gamma_1^* \rangle_r. \end{aligned} \tag{6}$$

Except in the special case $\Gamma_1^* = \Gamma_1 = \Gamma$, the 3-*j* symbol $\{(13), \Gamma_1^*\, \Gamma\, \Gamma_1\}_{rt}$ can be chosen to be $\{\Gamma_1^*\, \Gamma\, \Gamma_1\, r\}\delta_{rt}$ where the 3-*j* phase $\{\Gamma_1^*\, \Gamma\, \Gamma_1\, r\} = \pm 1$. Thus if $\Gamma_1 = \Gamma_1^*$

and if the 3-j phase can be chosen the same for all r we have

$$\langle \Gamma_1\, a_1^*\, \gamma_1^*\, i_1 | T^{n\,\alpha\Gamma}_{\ a0} | \Gamma_1\, a_1^*\, \gamma_1^*\, i_1 \rangle = \{\Gamma_1\,\Gamma_1\}\{\Gamma_1\,\Gamma\,\Gamma_1\,1\} \langle \Gamma_1\, a_1\, \gamma_1\, i_1 | T^{n\,\alpha\Gamma}_{\ a0} | \Gamma_1\, a_1\, \gamma_1\, i_1 \rangle \tag{7}$$

and we see that symmetries may exist among the eigenvalues. This equation can only be true in the special case $\Gamma_1 = \Gamma$ if Γ is a simple phase representation, i.e. the Kronecker cube $\Gamma\times\Gamma\times\Gamma$ does not contain the identity irrep in the mixed symmetry part (Butler and King 1974).

Because of this simple result we should not be surprised at the symmetries appearing in the tables of Judd *et al* (1974), especially when bearing in mind Derome's (1967) proof that SU(3) is a simple phase group.

Further, we can deduce from equation (7) that if an invariant is to resolve the branching multiplicity then it must do so in a definite manner. For example if $\gamma_1 = \gamma_1^*$ and $\{\Gamma_1\,\Gamma_1\}\{\Gamma_1\,\Gamma\,\Gamma_1\,1\} = +1$ then the multiplicity index must be self-contragredient whereas if there is a phase change it cannot unless the eigenvalue is zero. The equations for the sum of the eigenvalues and the sum of their moduli squared ensure in some cases that the desired resolution is made. Thus if $\{\Gamma_1\,\Gamma_1\}\{\Gamma_1\,\Gamma\,\Gamma_1\,1\} = -1$ then the branching multiplicity must be resolved, at least up to multiplicities of three, and the eigenvalues will occur in + and − pairs, and a zero if the multiplicity is odd. This is, of course, only true if the Kronecker product condition is satisfied.

To date, a proof of complete resolution is still lacking.

4. Hermiticity

It is desirable to use Hermitian operators for labelling purposes since their eigenvalues are then real and their eigenvectors can be chosen to be orthogonal even when there is degeneracy among the eigenvalues. We wish to know whether it is always possible to choose our invariants to be Hermitian and still retain our various conventions, especially that of Butler's (1975) 'sensible' phase for the 3-jm symbols. To investigate this we note that if an invariant is Hermitian then its matrix elements must be related by

$$\langle \Gamma_1\, a_1\, \gamma_1\, i_1 | T^{n\,\alpha\Gamma}_{\ a0} | \Gamma_2\, a_2\, \gamma_2\, i_2 \rangle = \langle \Gamma_2\, a_2\, \gamma_2\, i_2 | T^{n\,\alpha\Gamma}_{\ a0} | \Gamma_1\, a_1\, \gamma_1\, i_1 \rangle^*. \tag{8}$$

The right-hand side of equation (8) we can evaluate using equation (1) and applying the Derome–Sharp lemma to the 3-jm factor (Butler and Wybourne 1976, equation (38)). Use of permutational symmetries and other properties indicates that it is unlikely that an equality exists. However, it can be seen that the following are a sufficient set of conditions for the invariant to be chosen Hermitian:

(*a*) $$\begin{pmatrix} \Gamma_1^* & \Gamma^* & \Gamma_2 \\ a_1^*\,\gamma_1^* & a^*0 & a_2\,\gamma_2 \end{pmatrix}^r = \begin{pmatrix} \Gamma_1^* & \Gamma & \Gamma_2 \\ a_1^*\,\gamma_1^* & a0 & a_2\,\gamma_2 \end{pmatrix}^r.$$

This is normally only true if $\Gamma = \Gamma^*$ and $a = a^*$ but in practice can usually be readily satisfied. (Anyway, we note that when the reduction $\Gamma \to 0$ is not multiplicity-free then the invariants $T^{n\,\alpha\Gamma}_{\ a0}$ are not in general suitable as labelling operators because of the symmetry considerations of the last section.)

(*b*) The reduced matrix element is either pure real or pure imaginary, i.e.

$$\langle\Gamma_1\|\mathbf{T}^{n\alpha\Gamma}\|\Gamma_1\rangle_r^* = \sigma\langle\Gamma_1\|\mathbf{T}^{n\alpha\Gamma}\|\Gamma_1\rangle_r$$

where $\sigma = \pm 1$.

(*c*)
$$\sigma\{\Gamma_1\,\Gamma_1\}\begin{pmatrix}\Gamma & \Gamma^* \\ a0 & a^*0\end{pmatrix}\{(13), \Gamma_1^*\,\Gamma^*\,\Gamma_1\}_{rt} = +\delta_{rt}$$

for every irrep Γ_1 of G.

While these conditions may appear rather stringent they can in fact be satisfied for several groups of interest.

5. Independence of the invariants

In contrast with classical invariant theory, the product and commutator of two invariant operators yield sums of operators of varying degrees in the generators (cf the proof by Judd *et al* (1974) of a finite integrity basis). It is obvious that these are also invariants and again that they belong to U. We wish to know what invariants will occur in such products or commutators.

The Wigner–Racah algebra may be used to find the product of two invariants, $T^{n_1}{}^{\alpha_1\Gamma_1}_{a_10}$ and $T^{n_2}{}^{\alpha_2\Gamma_2}_{a_20}$ say, by comparing their joint action on an arbitrary ket $|\Gamma_x\, a_x\, \gamma_x\, i_x\rangle$ with the action of other operators, $T^{n}{}^{\alpha\Gamma}_{a0}$. Recalling that the operators are linear we have

$$\begin{aligned}
&T^{n_1}{}^{\alpha_1\Gamma_1}_{a_10}T^{n_2}{}^{\alpha_2\Gamma_2}_{a_20}|\Gamma_x\, a_x\, \gamma_x\, i_x\rangle \\
&\quad= \sum_{\substack{a_y\gamma_yi_y\\ a_z\gamma_zi_z}} |\Gamma_x\, a_z\, \gamma_z\, i_z\rangle\langle\Gamma_x\, a_z\, \gamma_z\, i_z|T^{n_1}{}^{\alpha_1\Gamma_1}_{a_10}|\Gamma_x\, a_y\, \gamma_y\, i_y\rangle \\
&\quad\quad\times\langle\Gamma_x\, a_y\, \gamma_y\, i_y|T^{n_2}{}^{\alpha_2\Gamma_2}_{a_20}|\Gamma_x\, a_x\, \gamma_x\, i_x\rangle.
\end{aligned}\tag{9}$$

We can evaluate this expression using the Wigner–Eckart theorem and comparison with the action of $T^{n}{}^{\alpha\Gamma}_{a0}$ is then made by using a 6-*j* symbol (again we adhere to Butler's (1975) definitions). The result can be interpreted as

$$\begin{aligned}
&T^{n_1}{}^{\alpha_1\Gamma_1}_{a_10}T^{n_2}{}^{\alpha_2\Gamma_2}_{a_20} \\
&\quad= \sum_{s\Gamma a} |\Gamma|^{1/2}\begin{pmatrix}\Gamma & \Gamma^* \\ a0 & a^*0\end{pmatrix}\begin{pmatrix}\Gamma_1 & \Gamma_2 & \Gamma^* \\ a_10 & a_20 & a^*0\end{pmatrix}^s[\mathbf{T}^{n_1\alpha_1\Gamma_1}\mathbf{T}^{n_2\alpha_2\Gamma_2}]^{s\Gamma}_{a0}
\end{aligned}\tag{10}$$

where the $[\mathbf{T}^{n_1\alpha_1\Gamma_1}\mathbf{T}^{n_2\alpha_2\Gamma_2}]^{s\Gamma}_{a0}$ are tensor operators related to the $T^{n}{}^{\alpha\Gamma}_{a0}$ by

$$\sum_s [\mathbf{T}^{n_1\alpha_1\Gamma_1}\mathbf{T}^{n_2\alpha_2\Gamma_2}]^{s\Gamma}_{a0} = \sum_{n\alpha} T^{n}{}^{\alpha\Gamma}_{a0}\tag{11}$$

and possessing reduced matrix elements given by

$$\begin{aligned}
&\langle\Gamma_x\|[\mathbf{T}^{n_1\alpha_1\Gamma_1}\mathbf{T}^{n_2\alpha_2\Gamma_2}]^{s\Gamma}\|\Gamma_x\rangle_r \\
&\quad= \sum_{r_1r_2r_3s_1s_2} |\Gamma|^{1/2}\langle\Gamma_x\|\mathbf{T}^{n_1\alpha_1\Gamma_1}\|\Gamma_x\rangle_{r_1}\langle\Gamma_x\|\mathbf{T}^{n_2\alpha_2\Gamma_2}\|\Gamma_x\rangle_{r_2}\begin{Bmatrix}\Gamma_1 & \Gamma_2 & \Gamma^* \\ \Gamma_x & \Gamma_x & \Gamma_x\end{Bmatrix}_{s_1s_2r_3s} \\
&\quad\quad\times\{\Gamma^*\,\Gamma\}\{\Gamma_x\,\Gamma_x^*\}\{(12), \Gamma_1\,\Gamma_x^*\,\Gamma_x\}_{r_1s_1}\{(13), \Gamma_x\,\Gamma_2\,\Gamma_x^*\}_{r_2s_2}\{(123), \Gamma_x^*\,\Gamma\,\Gamma_x\}_{r_3r}.
\end{aligned}\tag{12}$$

A similar sort of result can be found for the commutator by interchanging the order of the product. Thus we find that

$$[T^{n_1\alpha_1\Gamma_1}_{a_1 0}, T^{n_2\alpha_2\Gamma_2}_{a_2 0}]$$
$$= \sum_{s\Gamma a} |\Gamma|^{1/2} \begin{pmatrix} \Gamma & \Gamma^* \\ a0 & a^*0 \end{pmatrix} \begin{pmatrix} \Gamma_1 & \Gamma_2 & \Gamma^* \\ a_1 0 & a_2 0 & a^* 0 \end{pmatrix}^s$$
$$\times ([\mathbf{T}^{n_1\alpha_1\Gamma_1}\mathbf{T}^{n_2\alpha_2\Gamma_2}]^{s\Gamma}_{a0} - \{\Gamma_1\,\Gamma_2\,\Gamma^*\,s\}[\mathbf{T}^{n_2\alpha_2\Gamma_2}\mathbf{T}^{n_1\alpha_1\Gamma_1}]^{s\Gamma}_{a0}) \tag{13}$$

where the reduced matrix elements of $[\mathbf{T}^{n_2\alpha_2\Gamma_2}\mathbf{T}^{n_1\alpha_1\Gamma_1}]^{s\Gamma}_{a0}$ may be deduced from equation (12) and the $T^{n\,\alpha\Gamma}_{\;\,a0}$ arising in the commutator are given by

$$\sum_{n\alpha} T^{n\,\alpha\Gamma}_{\;\,a0} = \sum_{s} ([\mathbf{T}^{n_1\alpha_1\Gamma_1}\mathbf{T}^{n_2\alpha_2\Gamma_2}]^{s\Gamma}_{a0} - \{\Gamma_1\,\Gamma_2\,\Gamma^*\,s\}[\mathbf{T}^{n_2\alpha_2\Gamma_2}\mathbf{T}^{n_1\alpha_1\Gamma_1}]^{s\Gamma}_{a0}). \tag{14}$$

(In these expressions the sum over n ranges at most from 0 to n_1+n_2.)

Unfortunately the summation over n and α means that the invariants which may arise are not uniquely determined. However, it is clear that we can regard some invariants as being polynomially dependent on others via such constructions. Of course, from any product or commutator we can only select one term as being dependent and we would normally choose that which is of highest degree in the generators and which transforms as the representation of greatest weight.

We point out that equations (10) and (13) require resolutions of both branching and product multiplicities. However, for the purpose of establishing the independence of the invariants we may make an arbitrary resolution of both such that the summation over either involves only one term. We note that this means of resolving the multiplicity would not in general yield orthogonal bases. If desired though, an orthogonal basis could be constructed via the Gram–Schmidt procedure.

Lastly we mention that redundancies may occur in eliminating independent invariants. For instance three different constructions might only yield two linearly independent invariants. Such redundancies must arise if there are more ways of constructing invariants transforming as the irrep Γ than is the dimension of the invariant subspace transforming as Γ since, if we already have a number of linearly independent invariants equal to the dimension of the invariant subspace then these are a basis for the subspace and any further invariants must be linear combinations of them.

6. The pentahedral subgroup of SO(4)

We come now to the task of applying the tensor operator method to a specific example. The one that we have chosen is the restriction of SO(4) to one of its finite subgroups, namely the pentahedral group. First let us briefly describe this group and the nature of the labelling problem.

A regular four-simplex is the four-dimensional analogue of the tetrahedron in three dimensions and the equilateral triangle in two dimensions. By virtue of this figure having five faces it is known as a pentahedron. We can construct a pentahedron in four-dimensional Euclidean space, E_4 by adjoining to a tetrahedron in three-dimensional Euclidean space, E_3 a fifth vertex in a new fourth dimension.

Thus it is elementary to show that if we begin with a tetrahedron having the x_3 axis an axis of three-fold symmetry then the five points

$$(0, 0, 0, 1), \quad (0, 0, \sqrt{\tfrac{15}{16}}, -\tfrac{1}{4}), \quad (\sqrt{\tfrac{5}{6}}, 0, -\sqrt{\tfrac{5}{48}}, -\tfrac{1}{4}),$$
$$(-\sqrt{\tfrac{5}{24}}, \sqrt{\tfrac{5}{8}}, -\sqrt{\tfrac{5}{48}}, -\tfrac{1}{4}) \quad \text{and} \quad (-\sqrt{\tfrac{5}{24}}, -\sqrt{\tfrac{5}{8}}, -\sqrt{\tfrac{5}{48}}, -\tfrac{1}{4})$$

are the vertices of a pentahedron lying on the unit hypersphere with centre at the origin. The inverted figure obtained by negating the fourth coordinate is also a solution. If we started instead with a tetrahedron have the x_1, x_2 and x_3 axes as axes of two-fold symmetry then we would find that the points

$$(0, 0, 0, 1), \quad \left(\frac{\sqrt{5}}{4}, \frac{\sqrt{5}}{4}, -\frac{\sqrt{5}}{4}, -\frac{1}{4}\right), \quad \left(\frac{\sqrt{5}}{4}, -\frac{\sqrt{5}}{4}, \frac{\sqrt{5}}{4}, -\frac{1}{4}\right),$$
$$\left(-\frac{\sqrt{5}}{4}, \frac{\sqrt{5}}{4}, \frac{\sqrt{5}}{4}, -\frac{1}{4}\right) \quad \text{and} \quad \left(-\frac{\sqrt{5}}{4}, -\frac{\sqrt{5}}{4}, -\frac{\sqrt{5}}{4}, -\frac{1}{4}\right)$$

are also the vertices of a pentahedron and again the inverted figure can be constructed from the same tetrahedron. Clearly there are an infinite number of ways of embedding a pentahedron in E_4.

It is not difficult to deduce a set of matrices which permute the vertices of a pentahedron amongst themselves. These symmetry operations, which are elements of SO(4), form a group isomorphic to the alternating group on five objects, A_5. It is this symmetry group which we call the pentahedral group P.

The symmetry group of an icosahedron (or a dodecahedron) in E_3 is also isomorphic to A_5 (Klein 1884). Now an icosahedron can also be embedded in E_4 simply by adjoining a constant fourth coordinate to each of its twelve vertices. The embedding of the corresponding icosahedral group, I in SO(4) is however distinct in that the branching rules are different for the two cases. We can show the two reductions schematically as follows:

$$\begin{array}{cc}
\mathrm{SO}(4) & \mathrm{SO}(4) \\
\downarrow & \big| \\
\mathrm{SO}(3)\times\mathrm{SO}(1) & \big| \\
\downarrow & \downarrow \\
(\mathrm{I}\times\mathrm{SO}(1))\cong \mathrm{A}_5 & \mathrm{P}\cong\mathrm{A}_5 \\
\downarrow & \downarrow \\
(\mathrm{T}\times\mathrm{SO}(1))\cong\mathrm{A}_4 & (\mathrm{T}\times\mathrm{SO}(1))\cong\mathrm{A}_4 \\
\text{icosahedron} & \text{pentahedron}
\end{array}$$

where SO(1) is the trivial group consisting only of the identity operation on the fourth coordinate. Obviously SO(3)×SO(1) is isomorphic to SO(3) and similarly for I× SO(1) and T×SO(1). Note that one group reduction can be performed via SO(3) while the other cannot and also that the same tetrahedral group, T can be chosen in both cases. We leave further discussion of the branching rules to the next section.

7. Wigner–Racah algebra for SO(4) ⊃ P

We label the irreps of SO(4) in the normal fashion by $[pq]$, where p and q are integers for true irreps and half-(odd) integers for spin irreps. The irreps are of dimension

$$|[pq]| = (p+1)^2 - q^2. \tag{15}$$

Wybourne and Butler (1969) have used a 2 : 1 homomorphism between SO(4) and the double binary full linear group GL(2), which results in the correspondences

$$[ab] \to \{a+b\}\{a-b\}' \tag{16a}$$

$$\{a\}\{b\}' \to [\tfrac{1}{2}(a+b), \tfrac{1}{2}(a-b)], \tag{16b}$$

along with the algebra of S-functions to obtain a formula for the reduction of the Kronecker products of SO(4). Their result is

$$[ab][cd] = \sum_{\alpha=0}^{t} \sum_{\beta=0}^{u} [a+c-\alpha-\beta, b+d-\alpha+\beta] \tag{17}$$

where t is the lesser of $(a+b)$ and $(c+d)$ and u is the lesser of $(a-b)$ and $(c-d)$.

Our notation for the irreps of P follows that of Griffith (1961) for the icosahedral group. Griffith has given the reduction of the Kronecker products for these irreps.

There are several ways of calculating the branching rules for SO(4)$\to$P. We have found the method of Backhouse and Gard (1974) to be a particularly simple one. They have noted an automorphism which they call $\sim$ (tilde) on the character ring of A_5 and have used this, along with the known branching rules for SO(3)$\to$I, to perform the reduction of the irreps of SO(4) to those of P. Their prescription is

$$[pq] \downarrow \mathrm{P} \equiv \widetilde{\left(\left[\frac{p+q}{2}\right] \downarrow \mathrm{I}\right)} \times \left(\left[\frac{p-q}{2}\right] \downarrow \mathrm{I}\right). \tag{18}$$

The effect of $\sim$ is simply to interchange T_1 for T_2 and E$'$ for E$''$. Thus we find for example that under SO(4)$\to$P

$$[42] \to \mathrm{A} + \mathrm{T}_1 + \mathrm{T}_2 + \mathrm{U} + 2\mathrm{V}$$

whereas under SO(4)$\to$SO(3)$\to$I, since under SO(4)$\to$SO(3)

$$[pq] \to [p] + [p-1] + [p-2] + \ldots + [|q|], \tag{19}$$

we have

$$[42] \to [4] + [3] + [2] \to \mathrm{T}_2 + 2\mathrm{U} + 2\mathrm{V}.$$

It is clear that since the branching rules are different in the two cases then the Wigner–Racah algebra is different, even though the groups are isomorphic. We point out that the branching multiplicity arising in SO(4)$\to$SO(3)$\to$I has been essentially resolved by us previously (Bickerstaff and Wybourne 1976) and emphasise that the pentahedral subgroup of SO(4), in which we are currently interested, poses a distinct labelling problem.

In order to apply the tensor operator technique we need to know the values of the 2-j and 3-j symbols and 2-jm factors that will arise. To begin with we note that SO(4) is simply reducible and therefore there is no multiplicity in the Kronecker products of its irreps and also the irreps are all self-contragredient, i.e. $[pq]^* = [pq]$.

Butler and King (1974) have shown that we may choose the 2-j symbol $\{[pq][pq]\}$ to be +1 for true irreps and −1 for spin irreps. Therefore we may write

$$\{[pq][pq]\} = (-1)^{2p}. \tag{20}$$

Because there is no product multiplicity, the 3-j symbol $\{\pi, [p_1q_1][p_2q_2][p_3q_3]\}_{11}$ can always be chosen +1 for even permutations and to be the 3-j phase $\{[p_1q_1][p_2q_2][p_3q_3]\}$ for odd permutations, even when the irreps are all equal. To obtain this phase we need only consider the case where two of the irreps are equal, $[p_1q_1]=[p_2q_2]$ say, and resolve the Kronecker square of this irrep into its symmetric and antisymmetric parts. This can be done via the plethysms $[p_1q_1]\otimes\{2\}$ and $[p_1q_1]\otimes\{1^2\}$ respectively. Consider the latter. Using the correspondence (16a) and the rules of plethysm we have

$$[p_1q_1]\otimes\{1^2\}\to(\{p_1+q_1\}\otimes\{1^2\})(\{p_1-q_1\}'\otimes\{2\})+(\{p_1+q_1\}\otimes\{2\})(\{p_1-q_1\}'\otimes\{1^2\}). \tag{21}$$

The plethysm $\{m\}\otimes\{2\}$ is given by

$$\{m\}\otimes\{2\}=\begin{cases}\{0\}+\{4\}+\{8\}+\ldots+\{2m\} & m \text{ even}\\ \{2\}+\{6\}+\{10\}+\ldots+\{2m\} & m \text{ odd}\end{cases} \tag{22}$$

and similarly we have

$$\{m\}\otimes\{1^2\}=\begin{cases}\{0\}+\{4\}+\{8\}+\ldots+\{2m-2\} & m \text{ odd}\\ \{2\}+\{6\}+\{10\}+\ldots+\{2m-2\} & m \text{ even.}\end{cases} \tag{23}$$

Using equations (22) and (23) in equation (21), expanding the terms and transforming back to irreps of SO(4) via the correspondence (16b) we obtain those irreps $[p'q']$ in the antisymmetric part of the Kronecker square. All other irreps in the Kronecker square must be contained in the symmetric part. The result divides the Kronecker square very neatly and allows us to choose the 3-j phase for both spin and true irreps to be

$$\{[p_1q_1][p_2q_2][p_3q_3]\}=(-1)^{p_1+p_2+p_3}. \tag{24}$$

(Note that the Kronecker product of spin irreps only contains true irreps and therefore the sum $p_1+p_2+p_3$ is always an integer.)

The only restriction on the phases of the 2-jm factors is their permutational symmetry relation (Butler and Wybourne 1976)

$$\begin{pmatrix}[pq] & [pq]\\ a\gamma & a^*\gamma\end{pmatrix}=\{[pq][pq]\}\{\gamma\gamma\}\begin{pmatrix}[pq] & [pq]\\ a^*\gamma & a\gamma\end{pmatrix} \tag{25}$$

where we have used the fact that the irreps of P are also self-contragredient. Now the true irreps of P are all orthogonal while the spin irreps are all symplectic (see Butler and King 1974 and, for instance, Smith and Wybourne 1967) and therefore we have that the 2-j symbol $\{\gamma\gamma\}$ for P is +1 for true irreps and −1 for spin irreps. We have already noted that the same choice can be made for SO(4) and since the branching rules for SO(4)→P yield only true irreps of P if the irrep of SO(4) is true and only spin irreps of P if the irrep of SO(4) is a spin irrep we can choose all 2-jm factors for SO(4)⊃P to be +1.

In order to obtain quantitative results we also need to know the 3-jm factors. However, these cannot be calculated without assuming a resolution of the branching multiplicity—which defeats our purpose. Therefore we shall transform to the canonical basis SO(4)⊃SO(3)⊃SO(2) for numerical work. The coupling theory for this chain is known (Biedenharn 1961) and the definition of the canonical tensor operators we employ is that of Wybourne (1970b).

For simply reducible groups, the value of the reduced matrix elements that one uses is immaterial as regards the labelling problem. It should suffice to say here merely that we have chosen them to be complex by including a factor $(\mathrm{i})^P$. This ensures that the invariant operators are always Hermitian.

8. Enumeration of the symmetric invariants

The six generators of SO(4) span the two irreps [11] and [1 − 1] of SO(4). Hence the invariant operators within the universal enveloping algebra of SO(4) transform as representations occurring in $([11]+[1-1])\otimes\{n\}$. We can evaluate this plethysm after first using the correspondence (16*a*) and the rules of plethysm to obtain

$$([11]+[1-1])\otimes\{n\}\to\sum_{m=0}^{n}(\{2\}\otimes\{m\})(\{2\}'\otimes\{n-m\}). \tag{26}$$

Then, substituting equation (22) into this expression, expanding, re-arranging terms and using the correspondence (16*b*) we arrive at the surprisingly simple result

$$([11]+[1-1])\otimes\{n\}=\begin{cases}\displaystyle\sum_{q=-p}^{p}\sum_{p=0}^{n/2}\tfrac{1}{2}(n+2-2p)[2p,2q] & n \text{ even}\\[2ex] \displaystyle\sum_{q=-[(2p+1)/2]}^{[(2p+1)/2]}\ \sum_{p=0}^{[(n-1)/2]}\tfrac{1}{2}(n+1-2p)[2p+1,2q] & n\text{ odd.}\end{cases} \tag{27}$$

We note that the symmetric parts of the Kronecker powers of $[11]+[1-1]$ only contain irreps $[pq]$ for which $p+q$ is even and that these occur in a complete and systematic fashion. Using the branching rules (18) it is now possible to write down all the nth-order scalars under P for any value of n.

An alternative method of enumerating the symmetric invariants is to note that under the restriction SO(4)→P the irreps [11] and [1 − 1] decompose as T_2 and T_1 respectively. Thus the plethysm $([11]+[1-1])\otimes\{n\}$ is equivalent to

$$(\mathrm{T}_1+\mathrm{T}_2)\otimes\{n\}=\sum_{m=0}^{n}(\mathrm{T}_1\otimes\{m\})(\mathrm{T}_2\otimes\{n-m\}) \tag{28}$$

which is easily evaluated by the method of Smith and Wybourne (1967). Reduction of the Kronecker products then yields the invariants directly. However, it requires a little more thought to derive the irreps of SO(4) under which they transform.

It is convenient at this stage to make a comment about the form of the Kronecker squares of SO(4) irreps. From equation (17) the Kronecker square is given by

$$[pq]^{\times 2}=\sum_{\alpha=0}^{p+q}\sum_{\beta=0}^{p-q}[2p-\alpha-\beta,2q-\alpha+\beta]. \tag{29}$$

Thus the irreps $[p'q']$ occurring in the Kronecker square are those for which

$$p'+q'=2(p+q)-2\alpha \tag{30}$$

and since $p+q$ and α are both always integers the sum $p'+q'$ is always even. Hence those irreps $[p'q']$ for which $p'+q'$ is odd can never be contained in the Kronecker square of any irrep $[pq]$ and therefore subgroup scalars symmetrised with respect to such an irrep could not be used as labelling operators, since their matrix elements would always be zero. This precisely coincides with those operators which cannot be constructed from the symmetric parts of the Kronecker powers of the generators of SO(4).

9. An integrity basis for pentahedral invariants

An invariant that can be resolved as a product or commutator of other invariants may possess unexpected relationships between its eigenvalues, but otherwise there is little reason for preferring an integrity basis member, ahead of other invariants, for labelling purposes. Nevertheless we shall attempt to find an integrity basis for the pentahedral invariants within the universal enveloping algebra of SO(4) so as to demonstrate the application of the tensor operator method outlined earlier.

Recall that we said that the method as given did not allow any precise statements to be made regarding the independence of invariants. However, we can still use it to make some good guesses. For instance the two sixth-order invariants $T^{6\alpha[40]}_{\ \ 0}$ and $T^{6\beta[40]}_{\ \ 0}$ are obviously just products of the fourth-order invariant $T^{4[40]}_{\ \ 0}$ with the two Casimir invariants $T^{2\alpha[00]}_{\ \ 0}$ and $T^{2\beta[00]}_{\ \ 0}$. We may proceed in a like manner to construct most of the other invariants as fully-stretched products of just a few remaining invariants, which we term elementary scalars. These we tabulate in table 1. Thus all invariants can be expressed as a fully-stretched polynomial in these elementary scalars.

The use of commutators considerably reduces the number of invariants which might be considered independent. We note that for SO(4) the coupled tensors $[\mathbf{T}^{n_1\alpha_1[p_1q_1]}\mathbf{T}^{n_2\alpha_2[p_2q_2]}]^{[pq]}_{a0}$ and $[\mathbf{T}^{n_2\alpha_2[p_2q_2]}\mathbf{T}^{n_1\alpha_1[p_1q_1]}]^{[pq]}_{a0}$ are equivalent and therefore the

Table 1. Elementary scalars for SO(4) ⊃ P.

Degree in the SO(4) generators	Irreps of SO(4) under which the elementary scalars transform	Total number of symmetric scalars	Number of elementary scalars
0	[00]	1	1
1	—	0	0
2	α[00], β[00]	2	2
3	—	0	0
4	[40], [4 ± 2]	6	3
5	—	0	0
6	[60], [6 ± 2], [6 ± 4], [6 ± 6]	17	7
7	[7 ± 1], [7 ± 3]	4	4
8	[8 ± 6]	36	2
9	[9 ± 1], [9 ± 3]*a*, [9 ± 3]*b*, [9 ± 5], [9 ± 7]	18	10
10	[10 ± 10]	74	2
11	[11 ± 7], [11 ± 9]	46	4
12	—	141	0
13	[13 ± 11]	102	2
14	—	246	0
15	[15 ± 15]	202	2
16	—	·406	0
17	—	358	0
18	—	661	0

commutation relation (13) simplifies to

$$[T^{n_1\alpha_1[p_1q_1]}_{\ \ a_1 0},\ T^{n_2\alpha_2[p_2q_2]}_{\ \ a_2 0}]$$
$$= \sum_{[pq]a} \sqrt{(p+q+1)(p-q+1)}\begin{pmatrix} [p_1q_1] & [p_2q_2] & [pq] \\ a_1 0 & a_2 0 & a^* 0 \end{pmatrix}$$
$$\times(1-(-1)^{p_1+p_2+p})[\mathbf{T}^{n_1\alpha_1[p_1q_1]}\mathbf{T}^{n_2\alpha_2[p_2q_2]}]^{[pq]}_{a0}. \tag{31}$$

Using the commutation relations together with some further, previously unused, products we are able to deduce that a minimum integrity basis (it is not unique) probably consists of the six operators $T^{4[40]}_{\ \ 0}$, $T^{4[42]}_{\ \ 0}$, $T^{4[4-2]}_{\ \ 0}$, $T^{6[60]}_{\ \ 0}$, $T^{6[66]}_{\ \ 0}$, $T^{6[6-6]}_{\ \ 0}$ and the two Casimir invariants. Further wittling down of the size of the integrity basis would involve constructing these operators from higher-order ones—a process which we would view with suspicion.

Although there is at present a lack of rigour associated with this technique it should be clear that it possesses great potential for providing a rapid and simple means of finding an integrity basis and is certainly worthy of some effort being aimed at its refinement.

10. The choice of labelling operators

Any SO(4) operator capable of resolving the branching multiplicity in the reduction SO(4)→P must not have all zero matrix elements within any module $[pq]$ for which branching multiplicity occurs. If the labelling operator is symmetrised with respect to the irrep $[p'q']$ of SO(4) this means that $[p'q']$ must be contained in the Kronecker square of $[pq]$. We wish to find what restrictions there are on the values of p' and q' in order that the condition

$$[pq]^{\times 2} \supset [p'q']$$

can be satisfied for (almost) any irrep $[pq]$. From the formula (29) for the Kronecker square we can deduce that we must have

$$0 \leqslant p'+q' \leqslant 2(p+q) \qquad \text{and} \qquad 0 \leqslant p'-q' \leqslant 2(p-q).$$

Now if $q=p$ or $q=-p$ then we can see that the only operators capable of resolving a branching multiplicity are those symmetrised with respect to the irreps $[p'p']$ or $[p'-p']$ respectively where $p' \leqslant 2p$. It is clear from the commutation relation (31) and the form of the Kronecker product that such a pair of operators will always commute. Sometimes one operator would perform the resolution, sometimes the other and sometimes both simultaneously.

However, the lowest-order symmetric invariants of this form are $T^{6[66]}_{\ \ 0}$ and $T^{6[6-6]}_{\ \ 0}$. It follows immediately from the above conditions that this pair of commuting operators does not suffice to resolve the labelling problem in all cases since the Kronecker squares of the irreps [40], [41], [4 − 1], [50], $[\frac{7}{2}\frac{1}{2}]$, $[\frac{7}{2}-\frac{1}{2}]$, $[\frac{7}{2}\frac{3}{2}]$, $[\frac{7}{2}-\frac{3}{2}]$, $[\frac{9}{2}\frac{1}{2}]$ and $[\frac{9}{2}-\frac{1}{2}]$ do not contain either the [66] irrep or the [6 − 6] irrep and yet they all exhibit branching multiplicity on reduction to irreps of P. The commuting symmetric invariants $T^{6[66]}_{\ \ 0}$ and $T^{6[6-6]}_{\ \ 0}$ may come remarkably close to completely resolving the labelling problem but they fail in these ten cases. Higher-order commuting pairs such as $T^{10[10\,10]}_{\ \ \ \ \ 0}$ and $T^{10[10-10]}_{\ \ \ \ \ \ 0}$, $T^{6[66]}_{\ \ \ 0}$ and $T^{10[10-10]}_{\ \ \ \ \ \ 0}$ etc fare even worse.

It is easy to determine what other symmetric invariants do satisfy the Kronecker product condition for these irreps. The only ones suitable in all cases are those transforming as [40] (in particular $T^{4[40]}_{\ \ \ 0}$) though certain pairs ($T^{4[42]}_{\ \ \ 0}$, $T^{4[4-2]}_{\ \ \ \ 0}$ and $T^{6[62]}_{\ \ \ 0}$, $T^{6[6-2]}_{\ \ \ \ 0}$) occur in such a way that one or the other of the pair is always present. None of these commute with $T^{6[66]}_{\ \ \ 0}$ and $T^{6[6-6]}_{\ \ \ \ 0}$ though. Hence we have demonstrated that it is not possible to resolve the labelling problem for $SO(4) \rightarrow P$ via a set of commuting invariants each of which transforms irreducibly under SO(4)!

Consider then linear combinations of irreducible tensors. It is immediately obvious that a single operator such as

$$aT^{4[40]}_{\ \ \ 0} + bT^{6[66]}_{\ \ \ 0} + cT^{6[6-6]}_{\ \ \ \ 0}$$

where a, b, c are coefficients, might alone suffice. (Note that this operator is not of homogeneous degree in the generators.) Other possibilities include

$$aT^{4[42]}_{\ \ \ 0} + bT^{4[4-2]}_{\ \ \ \ 0} + cT^{6[66]}_{\ \ \ 0} + dT^{6[6-6]}_{\ \ \ \ 0}$$

and

$$aT^{6[62]}_{\ \ \ 0} + bT^{6[6-2]}_{\ \ \ \ 0} + cT^{6[6-6]}_{\ \ \ \ 0} + dT^{6[6-6]}_{\ \ \ \ 0}.$$

In the event of a single such operator resolving the branching multiplicity it would be patently pointless searching for other operators which commute with it.

Let us pause for a moment to consider this new line of thought. We are reminded of perturbation theory and level splitting. If the symmetry group of some zero-order Hamiltonian was SO(4) and a perturbation term invariant under P was present, then this perturbation term could be expanded in terms of SO(4) irreducible tensors which were invariant under P. It could well have a form very similar to one of the proposed labelling operators. In the absence of accidental degeneracy, such a perturbation Hamiltonian would fully resolve the branching multiplicities. This suggests that a single linear combination of irreducible tensors is indeed the best approach to a resolution of the branching multiplicity.

To test our hypothesis we calculate some of the eigenvalues of the first operator proposed. The transformation coefficients of the irreducible tensors may be readily calculated once it is noticed that the same tetrahedral group may be embedded in both chains $SO(4) \supset P$ and $SO(4) \supset SO(3) \supset I$. We know the transformation coefficients for the tetrahedral invariants (Bickerstaff and Wybourne 1976) and since the pentahedral invariants must be linear combinations of tetrahedral invariants we can deduce their expansions in the canonical basis by diagonalising an arbitrary linear combination and adjusting the coefficients so as to force the correct degeneracy. The easiest case is to diagonalise $T^{4[42]}_{\ \ \ 0}$ within the module [21]. We obtain two solutions, indicative of two possible orientations of the same tetrahedron within the pentahedron. A consistent set of transformation coefficients for all the invariants may be calculated by first deducing the form of the antisymmetric invariant,

$$T^{3[30]}_{\ \ \ 0} \simeq \pm i\sqrt{6}\,T^{[30]0}_{\ \ \ \ \ 0} + i\sqrt{5}\,(T^{[30]3}_{\ \ \ \ \ 2} - T^{[30]3}_{\ \ \ \ \ -2})$$

(note that it has zero matrix elements) and after choosing an embedding, performing coupling calculations in the canonical basis to obtain the other invariants. Thus we find that we may choose

$$
\begin{aligned}
&aT^{4[40]}_{\;\,0} + bT^{6[66]}_{\;\,0} + cT^{6[6-6]}_{\;\,0} \\
&\quad \simeq \frac{24\sqrt{5}}{7} T^{[40]0}_{\;\;\;\,0} + \frac{12\sqrt{15}}{7} (T^{[40]3}_{\;\;\;\,2} - T^{[40]3}_{\;\;\;\,-2}) - \frac{6\sqrt{70}}{7} T^{[40]4}_{\;\;\;\,0} \\
&\quad - \frac{30}{7} (T^{[40]4}_{\;\;\;\,4} + T^{[40]4}_{\;\;\;\,-4}) + \frac{2\sqrt{77}}{7} T^{[66]6}_{\;\;\;\,0} - \sqrt{33} (T^{[66]6}_{\;\;\;\,2} + T^{[66]6}_{\;\;\;\,-2}) \\
&\quad - \sqrt{22} (T^{[66]6}_{\;\;\;\,4} + T^{[66]6}_{\;\;\;\,-4}) + \sqrt{15} (T^{[66]6}_{\;\;\;\,6} + T^{[66]6}_{\;\;\;\,-6}) + \frac{2\sqrt{77}}{7} T^{[6-6]6}_{\;\;\;\;\;\,0} \\
&\quad + \sqrt{33} (T^{[6-6]6}_{\;\;\;\;\;\,2} + T^{[6-6]6}_{\;\;\;\;\;\,-2}) - \sqrt{22} (T^{[6-6]6}_{\;\;\;\;\;\,4} + T^{[6-6]6}_{\;\;\;\;\;\,-4}) - \sqrt{15} (T^{[6-6]6}_{\;\;\;\;\;\,6} + T^{[6-6]6}_{\;\;\;\;\;\,-6}).
\end{aligned}
$$

Some selected eigenvalues of this operator have been calculated and are given in table 2.

Table 2. Selected eigenvalues of $T^{4[40]}_{\;\,0} + T^{6[66]}_{\;\,0} + T^{6[6-6]}_{\;\,0}$.

SO(4) module	Eigenvalues	Degeneracy
[61]	−159734·150	3
	−159731·951	4
	−159675·655	5
	48982·045	5
	49427·571	3
	50578·815	4
	51392·835	3
	52070·494	5
	53357·310	3
	54305·744	1
	56822·249	4
	57635·687	5
	58874·749	3
[70]	−319392·7534	4
	−112177·2016	4
	−111486·9341	5
	−106616·0522	6
	−101817·6219	5
	−100872·9892	4
	100830·1933	5
	100874·0939	4
	102192·0941	6
	104791·4219	5
	109656·7138	5
	110506·9598	4
	113968·0169	6
	117114·3445	1
$[\frac{7}{2}\frac{1}{2}]$	−822·85714	6
	0·00000	4
	329·14286	8
	1152·00000	2

We see that some of the degeneracies are higher than expected but are still consistent with a resolution of the branching multiplicity. In fact the pattern of the degeneracies indicates that the same eigenvalue is occurring for different irreps rather than for different multiplicity labels.

The permutational symmetry of the 3-*jm* factors does not give rise to symmetries in the eigenvalues of this operator. However we could use an operator based on the pair $T^{15[15\,15]}_{0}$ and $T^{15[15\,-15]}_{0}$ (which would include terms such as $T^{7[7\,1]}_{0}$, $T^{7[7\,-1]}_{0}$, $T^{7[7\,3]}_{0}$ and $T^{7[7\,-3]}_{0}$) in which case we would obtain a resolution of the multiplicity for which the eigenvalues occur in + and − pairs and zeros.

11. Conclusions

We have pointed out that labelling operators for subgroups of compact Lie groups can be expressed in terms of irreducible tensors. Use of the irreducible tensor method admits simple means of enumerating invariants, predicting symmetries and choosing between various labelling operators.

By considering the pentahedral subgroup of SO(4) we have been able to demonstrate that the branching multiplicity cannot be resolved by a commuting set of irreducible tensors. Our method suggests that a single linear combination of irreducible tensors ought to resolve the labelling problem, provided the linear combination is sufficiently complicated. We conclude that the standard approach to labelling problems, via a set of mutually commuting operators is both inappropriate (except where the Hilbert space is a tensor product space) and not generally feasible.

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