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Integrity bases, invariant operators and the state labelling problem for finite subgroups of SO_3

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Abstract. The construction of integrity bases and invariant operators for the finite subgroups of SO_3 is outlined. The integrity bases are realized in terms of rotationally invariant sets of kets and the invariant operators in terms of irreducible tensorial sets. A building-up principle is developed for integrity bases and invariant operators and the latter used to complete the state labelling for the non-canonical subgroup chains. The invariant operators are applied to the symmetry adaption of Gel'fand states and to the study of coupling and transformation coefficients.

1. Introduction

A homogeneous polynomial $P_G^m(\boldsymbol{\alpha})$ of degree m in the n variables $\alpha_1, \alpha_2, \ldots, \alpha_n$ is said to be an *invariant* of a group G if for all group transformations $T(g)$ $(g \in G)$ we have

$$P_G^m[T(g)\boldsymbol{\alpha}] \equiv P_G^m(\boldsymbol{\alpha}).$$

A fundamental problem in the theory of invariants is to determine the minimal set $P_G[\boldsymbol{\alpha}]$ of invariant polynomials associated with a given group G in terms of which all other invariant polynomials may be generated. Such a minimal set of invariants is said (Weyl 1946) to constitute an *integral rational basis* or *integrity basis*. The integrity basis can be shown to be finite for any connected semi-simple compact Lie group (Judd *et al* 1974).

The determination of the numbers and degrees of the invariant polynomials constituting the integrity basis goes back to the generating functions of Molien (1897). In the particular case of the proper rotation group SO_3 we are initially interested in polynomials in the three spatial variables (x, y, z) invariant under the action of a subgroup of SO_3. The numbers and degrees of the invariant polynomials in (x, y, z) have been determined by Meyer (1954) for all the crystallographic point groups and for the non-crystallographic icosahedral group.

Explicit integrity bases for the crystallographic point groups have been given by Döring (1958), Döring and Simon (1960, 1961), Smith *et al* (1963, 1964) and Killingbeck (1972). McLellan (1974) has considered invariant polynomial functions of a symmetric second-order tensor while Kopsky (1975) has investigated Abelian crystal point groups.

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The choice of an integrity basis for a given group G is not unique. Different integrity bases are associated with the various subgroups H of G. Further, a given subgroup H of G may often be embedded in G in several different ways giving rise to different integrity bases. In many cases there is value in constructing integrity bases symmetrized with respect to the various subgroups of a given group G. For example, we may construct integrity bases for the icosahedral group from those found for the subgroups D_5, $T \supset D_2$ or $T \supset C_3$.

The representations $D^{(J)}$ of SO_3 are generally reducible upon restriction to a finite rotation group G. The reduction of the representation $D^{(J)}$ is often not multiplicity free. For example, under the restriction $SO_3 \to T$ we have for $J = 6$ (Koster *et al* 1963)

$$D^{(6)} \to 2\Gamma_1 + \Gamma_2 + \Gamma_3 + 3\Gamma_4.$$

In these cases the eigenvalues $J(J+1)$ of the Casimir invariant $\boldsymbol{J}^2$ of SO_3 together with the representation labels Γ_i of the tetrahedral group T do not supply a sufficient set of labels to distinguish states belonging to repeated representations of T. Following an argument due to Racah (1964) it is apparent that we are missing one labelling operator, say X. The Hermitian operator X may be constructed as a polynomial in the three generators $J_\pm$, J_z of the enveloping algebra of SO_3 that is invariant under the relevant finite subgroup G of SO_3. This operator, while not a scalar with respect to SO_3, will necessarily commute with the Casimir invariant $\boldsymbol{J}^2$ of SO_3. The eigenvalues of the invariant operator X can be used to supply the missing label and thus systematically distinguish the non-multiplicity free reductions.

The construction of invariant operators is closely related to that of constructing the integrity basis of the corresponding group. The invariant operators associated with a group G will be homogeneous polynomials in the group generators $J_\pm$, J_z and may be constructed so as to be associated with a particular representation $D^{(J)}$ of SO_3 and will be designated as $X_G^{(J)}$ with J being a non-negative integer. In this case invariant polynomials of degree J can be placed in one to one correspondence with the invariant operators $X_G^{(J)}$. However, due to the noncommutability of the group generators the minimal set of invariant operators will generally be smaller than that of the integrity basis of invariant polynomials. Indeed in our case the entire set of invariant operators can always be generated by $\boldsymbol{J}^2$ and any two of the invariant operators, say $X_G^{(J_1)}$ and $X_G^{(J_2)}$.

Considerable advantages accrue in representing the integrity bases in terms of functions that transform under rotations like spherical harmonics and the operators in terms of spherical tensor operators. The relationship between the invariant functions and invariant operators becomes very close and leads to considerable simplifications.

In this paper we first realize a set of kets $|kq\rangle$ in terms of homogeneous polynomials of degree k in the variables $x_\pm/r$, z/r where

$$x_\pm = \mp\frac{1}{\sqrt{2}}(x \pm \mathrm{i}y).$$

These kets are constructed from the elementary kets $|10\rangle$, $|1\pm1\rangle$ by a building-up process based on standard angular momentum coupling theory (Butler 1975). Next a set of irreducible tensor operators $T_q^{(k)}(\boldsymbol{J})$ are realized in terms of polynomials in $J_\pm$, J_z and constructed by an analogous building-up process. The commutation and coupling properties of these operators are then developed and the expressions for the tensor operator matrix elements in the angular momentum basis $|JM\rangle$ given.

A building-up principle for integrity bases and invariant operators is formulated to permit the systematic generation of higher-order invariant kets or operators from the lowest-order non-trivial invariant ket or operator. This systematic method is applied first to the cyclic and dihedral groups and then successively to the tetrahedral, octahedral and icosahedral groups paying special attention in these latter cases to the relevant subgroup structures.

The application of the invariant operators to the solution of the state labelling problem is illustrated by an example. The invariant operators can play an important role in the construction of symmetry adapted states. Particular application is given here to the symmetry adaption of Gel'fand states (Gel'fand and Tsetlin 1950a, b) making contact with recent work on the use of Gel'fand states in atomic (Patera 1972, Harter 1973, Drake *et al* 1975) and molecular (Paldus 1975) physics.

Diagonalization of the invariant operators $X_G^{(J)}$ in an angular momentum basis $|JM\rangle$ yields a symmetry adapted basis and the elements of the diagonalizing matrix are the transformation coefficients (Butler 1975) that take us from one basis into another. This leads us finally to discuss some of the properties of coupling coefficients and transformation coefficients and their systematic computation. The extension of the methods outlined in this paper for SO_3 and its subgroups to the other group structures is briefly considered.

2. Angular momentum basis states

The angular momentum operators $J_\pm$ and J_z define the enveloping algebra of the group SO_3. The kets $|kq\rangle$ where k is a non-negative integer and $q=-k, -k+1, \ldots, k$ will form a rotationally invariant set if (Edmonds 1957)

$$J_z|kq\rangle = q|kq\rangle; \qquad J_\pm|kq\rangle = [k(k+1)-q(q\pm 1)]^{1/2}|kq\pm 1\rangle. \tag{1}$$

A pair of kets $|k_1q_1\rangle$, $|k_2q_2\rangle$ may be coupled together to form coupled kets $|kq\rangle$ by writing

$$|k_1q_1\rangle|k_2q_2\rangle = \sum_{kq}(-1)^{k_1-k_2+q}(2k+1)^{1/2}\begin{pmatrix} k_1 & k_2 & k \\ q_1 & q_2 & -q \end{pmatrix}|(k_1k_2)kq\rangle \tag{2}$$

and conversely

$$|(k_1k_2)kq\rangle = \sum_{q_1q_2}(-1)^{k_1-k_2+q}(2k+1)^{1/2}\begin{pmatrix} k_1 & k_2 & k \\ q_1 & q_2 & -q \end{pmatrix}|k_1q_1\rangle|k_2q_2\rangle. \tag{3}$$

These two relations permit the systematic construction of arbitrary kets from the elementary kets $|10\rangle$, $|1\pm 1\rangle$.

The operators $J_\pm$, J_z may be realized in terms of (x, y, z) by writing

$$J_z = -\mathrm{i}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right); \qquad J_\pm = -\mathrm{i}\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right) \mp \mathrm{i}\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right). \tag{4}$$

The elementary kets then have the realization

$$|10\rangle \equiv z/r \qquad |1\pm 1\rangle \equiv x_\pm/r. \tag{5}$$

It follows from (3) that the simplest rank k kets are the kth order stretched kets

$$|k\pm k\rangle = x_\pm^k/r^k. \tag{6}$$

An arbitrary kth order ket $|kq\rangle$ can be generated either by systematic application of the raising or lowering operators $J_\pm$ to $|k \pm k\rangle$ as defined in (6) or by a building-up principle based on (5) and (3). Hence every ket $|kq\rangle$ can be realized as a polynomial in (x, y, z). The normalization of kets is fixed by the choice made in (5). We note that

$$|kq\rangle^* = (-1)^q |k -q\rangle. \tag{7}$$

We shall see shortly that the kets $|kq\rangle$ play a fundamental role in constructing integrity bases for finite subgroups of SO_3.

3. Irreducible tensorial sets

An irreducible spherical tensorial set $\boldsymbol{T}^{(k)}$ has $2k+1$ members $T_q^{(k)}$ with $q = -k, -k+1, \ldots, k$ which satisfy the commutation relations

$$[J_z, T_q^{(k)}] = qT_q^{(k)}; \qquad [J_\pm, T_q^{(k)}] = [k(k+1) - q(q\pm 1)]^{1/2} T_{q\pm 1}^{(k)}. \tag{8}$$

Comparison of (1) and (8) shows the well known similarity of kets and operators. The operators, like the kets, admit various realizations. For our purposes we realize the tensor operators in terms of polynomials in $J_\pm, J_z$. These operators will automatically be diagonal in the eigenvalues of $\boldsymbol{J}^2$.

The elementary tensor operators are defined as

$$T_0^{(1)} = J_z \qquad T_{\pm 1}^{(1)} = \mp \frac{1}{\sqrt{2}} J_\pm \tag{9), (10}$$

and we readily find that we may realize

$$T_{\pm k}^{(k)} = (T_{\pm 1}^{(1)})^k. \tag{11}$$

An arbitrary tensor operator component $T_q^{(k)}$ can be constructed as a polynomial in the angular momentum operators by application of the raising or lowering operators to (11) via (8). Alternatively, we may make use of the building up principle via

$$T_{q_1}^{(k_1)} T_{q_2}^{(k_2)} = \sum_{kq} (-1)^{k_1 - k_2 + q} (2k+1)^{1/2} \begin{pmatrix} k_1 & k_2 & k \\ q_1 & q_2 & -q \end{pmatrix} [\boldsymbol{T}^{(k_1)} \boldsymbol{T}^{(k_2)}]_q^{(k)} \tag{12}$$

where (Schwinger 1952, see also Biedenharn and Van Dam 1965)

$$[\boldsymbol{T}^{(k_1)} \boldsymbol{T}^{(k_2)}]_q^{(k)} = \frac{\langle J \| [T^{(k_1)} T^{(k_2)}]^{(k)} \| J \rangle}{\langle J \| T^{(k)} \| J \rangle} T_q^{(k)} \tag{13}$$

and (Judd 1963)

$$\langle J \| [T^{(k_1)} T^{(k_2)}]^{(k)} \| J \rangle = (-1)^{2J+k} (2k+1)^{1/2} \begin{Bmatrix} k_1 & k_2 & k \\ J & J & J \end{Bmatrix} \langle J \| T^{(k_1)} \| J \rangle \langle J \| T^{(k_2)} \| J \rangle. \tag{14}$$

The reduced matrix elements are given by (Buckmaster *et al* 1972)

$$\langle J \| T^{(k)} \| J \rangle = k! \left(\frac{(2J+k+1)!}{2^k (2k)! (2J-k)!} \right)^{1/2}. \tag{15}$$

It is important to note that (13) is J-dependent as indeed noted by Schwinger (1952). The exception is where $k = k_1 + k_2$, then

$$[\boldsymbol{T}^{(k_1)} \boldsymbol{T}^{(k_2)}]_q^{(k_1+k_2)} \equiv T_q^{(k_1+k_2)}. \tag{16}$$

The polynomial expansions in $J_\pm$, J_z for $T_q^{(k)}$ with $k=0$ to 7 have been given by Buckmaster *et al* (1972). In actual practice the detailed expansions are of little interest since the matrix elements of $T_q^{(k)}$ can be readily evaluated using the Wigner–Eckart theorem (Judd 1963) giving in this case

$$\langle \alpha JM|T_q^{(k)}|\alpha' J'M'\rangle = \delta_{\alpha\alpha'}\delta_{JJ'}(-1)^{J-M}\begin{pmatrix} J & k & J \\ -M & q & M' \end{pmatrix}\langle J\|T^{(k)}|J\rangle. \tag{17}$$

The operators $T_q^{(k)}$ do not in general commute, rather (Schwinger 1952, see also Biedenharn and Van Dam 1965)

$$[T_{q_1}^{(k_1)}, T_{q_2}^{(k_2)}] = \sum_{kq}(2k+1)^{1/2}\begin{pmatrix} k_1 & k_2 & k \\ q_1 & q_2 & -q \end{pmatrix}(-1)^{k_1-k_2+q}[1-(-1)^{k_1+k_2+k}][\boldsymbol{T}^{(k_1)}\boldsymbol{T}^{(k_2)}]_q^{(k)}. \tag{18}$$

4. Building-up principle for integrity bases and invariant operators

The properties of integrity bases are closely related to those of coupling transformation coefficients. A basis ket that is invariant under a subgroup G of SO_3 may be designated as $|J\alpha\Gamma_1\rangle$ where Γ_1 is the identity representation of G and α is a multiplicity label for those cases where Γ_1 occurs more than once in the reduction $SO_3 \to G$. These invariant kets may be formally expanded in terms of the standard angular momentum kets $|JM\rangle$ by writing

$$|J\alpha\Gamma_1\rangle = \sum_M |JM\rangle\langle JM|J\alpha\Gamma_1\rangle \tag{19}$$

where the coefficients of the expansion are transformation coefficients that couple the two bases (Kaplan 1962a, b, Moshinsky and Devi 1969).

An invariant ket $|J\alpha\Gamma_1\rangle$ can be constructed from other invariant kets, say $|J_1\alpha_1\Gamma_1\rangle$ and $|J_2\alpha_2\Gamma_1\rangle$, by noting that

$$\sum_\alpha \langle JM|J\alpha\Gamma_1\rangle\langle J\alpha\Gamma_1|J_1\alpha_1\Gamma_1; J_2\alpha_2\Gamma_1\rangle$$
$$= \sum_{M_1,M_2}\langle JM|J_1M_1; J_2M_2\rangle\langle J_1M_1|J_1\alpha_1\Gamma_1\rangle\langle J_2M_2|J_2\alpha_2\Gamma_1\rangle. \tag{20}$$

The right-hand side of (20) involves the transformation coefficients used to construct the kets $|J_1\alpha_1\Gamma_1\rangle$ and $|J_2\alpha_2\Gamma_1\rangle$ and angular momentum Clebsch–Gordan coefficients (Rotenberg *et al* 1959). The left-hand side of (20) involves a coupling coefficient for $SO_3 \supset G$ and the desired transformation coefficient for use in (19). The properties and calculation of the relevant coupling coefficients have been considered elsewhere (Butler 1975, Butler and Wybourne 1976a, b). We follow the notation of Butler (1975).

Equation (20) may be usefully rewritten in terms of the more symmetrical $1jm$ and $3jm$ symbols (Butler 1975) to give

$$\sum_{\alpha,\alpha'}(J)\alpha\Gamma_1, \alpha'\Gamma_1\begin{pmatrix} J_1 & J_2 & J \\ \alpha_1\Gamma_1 & \alpha_2\Gamma_1 & \alpha'\Gamma_1 \end{pmatrix}\langle JM|J\alpha\Gamma_1\rangle$$
$$= \sum_{M_1,M_2}(-1)^{J_1-J_2+M}\begin{pmatrix} J_1 & J_2 & J \\ M_1 & M_2 & -M \end{pmatrix}\langle J_1M_1|J_1\alpha_1\Gamma_1\rangle\langle J_2M_2|J_2\alpha_2\Gamma_1\rangle \tag{21}$$

where $M = M_1 + M_2$.

The above results give an alternative approach to the usual integrity basis constructions and are particularly useful for calculating the higher-order invariants for the cubic and icosahedral groups. In these cases we can systematically construct higher-order invariant symmetrized kets from lower-order invariant kets.

It is commonly stated that any polynomial invariant of a group G can be expressed as a polynomial in the integrity basis but the actual procedure for resolving a given polynomial invariant into that of the integrity basis is usually avoided. Similar remarks hold for the converse problem of resolving an arbitrary polynomial in the integrity basis into independent polynomial invariants of fixed orders. Both problems are amenable to a systematic, though often tedious, solution starting with equations such as (18) to (21). Specific examples will be given when we come to discuss the octahedral group.

The transformation properties of basis functions and operators are closely related (Judd 1963, Butler 1975) and the building-up process can be carried over to invariant operators directly with the one important difference that the resolution of the product of two operators is normally J-dependent as a consequence of (13). This is of little consequence provided we work within a fixed J-manifold.

5. Integrity bases for the cyclic and dihedral groups

The cyclic groups C_n are Abelian and involve n pure rotations about an n-fold axis. We shall choose this axis as the z axis. The dihedral groups D_n are formed from C_n by adding a 2-fold rotation perpendicular to the z axis to give a group containing $2n$ elements. We seek integrity bases where each member of a given set can be associated with a particular J value associated with the SO_3 Casimir invariant $\boldsymbol{J}^2$. We further demand that our invariants be Hermitian.

The invariants for a given group C_n may be constructed for the $|JM\rangle$ kets by standard application of the rotation operators of C_n to the kets (Bradley and Cracknell 1972, Buckmaster *et al* 1972). The integrity basis for a given $C_n (n>1)$ involves just four members and may be chosen as

$$C_n: \qquad |00\rangle, |10\rangle, (|nn\rangle+(-1)^n|n-n\rangle), \mathrm{i}[|nn\rangle-(-1)^n|n-n\rangle] \tag{22}$$

where

$$|00\rangle = \frac{x^2+y^2+z^2}{r^2} = 1. \tag{23}$$

The special case of C_1 is covered by deleting the first member in (22). The integrity bases for the dihedral groups D_n each involve four members which we may choose as $(n \geqslant 2)$

$$D_n: \qquad |00\rangle, |20\rangle, (|nn\rangle+(-1)^n|n-n\rangle); \mathrm{i}[|n+1n\rangle-(-1)^n|n+1-n\rangle]. \tag{24}$$

It is a simple matter to see that if the above kets are realized in terms of polynomials in (x, y, z) as in § 2 then all the polynomial invariants for C_n and D_n can be expressed as polynomials in the polynomial invariants of (22) and (24) respectively.

Alternative integrity basis for C_n and D_n can be defined by taking suitable linearly independent combinations of the members of a given integrity basis. Our bases differ from those of Killingbeck (1972) due to our requirement that each member of the set transforms under SO_3 according to a particular J value. An inconsistency in Killingbeck's bases for C_3 and D_3 is noted.

6. Invariant operators for the cyclic and dihedral groups

The construction of invariant operators for the cyclic and dihedral groups follow immediately from recognizing the similarity under transformations of kets and operators. Indeed we need simply note the correspondence (Judd 1963)

$$|kq\rangle \leftrightarrow T_q^{(k)} \tag{25}$$

where the $T_q^{(k)}$ are here realized in terms of polynomials in the generators $J_\pm$, J_z of SO_3 to give for

$$C_n: \qquad T_0^{(0)},\ T_0^{(1)},\ T_n^{(n)}+(-1)^n T_{-n}^{(n)},\ \mathrm{i}[T_n^{(n)}-(-1)^n T_{-n}^{(n)}] \tag{26}$$

and for

$$D_n: \qquad T_0^{(0)},\ T_0^{(2)},\ T_n^{(n)}+(-1)^n T_{-n}^{(n)},\ \mathrm{i}[T_n^{(n+1)}-(-1)^n T_{-n}^{(n+1)}] \tag{27}$$

where

$$T_0^{(0)} \propto \boldsymbol{J}^2 = (\surd 3)[\boldsymbol{T}^{(1)}\boldsymbol{T}^{(1)}]_0^{(0)}. \tag{28}$$

However, there is an important difference, the operators $T_q^{(k)}$ generally do not commute. The commutator of two invariants is itself an invariant and hence all four members of the set of invariant operators associated with a given group are not independent. The minimal set of invariant operators may always be chosen as consisting of $T_0^{(0)}$ and any two of the remaining invariant operators. This set of three independent invariant operators suffice to generate all other invariant operators. Clearly $T_0^{(0)}$ commutes with all other invariant operators.

7. Integrity bases and invariant operators for the tetrahedral group

The tetrahedral group T is made up of the pure rotations of the tetrahedron. The groups D_2 and C_3 occur as subgroups of T and permit the construction of two distinct group–subgroup bases according to $T \supset D_2$ or $T \supset C_3$. It follows from Meyer (1954), or simple character theory, that the invariant polynomials occuring in both integrity bases are of degree 0, 3, 4 and 6. The third-order invariant of D_2 is also a third-order invariant for T since upon restriction from $J=3$ of SO_3 both groups yield the identity representation just once. This is not the case for $T \supset C_3$.

An integrity basis for $T \supset C_3$ may be obtained from one for $T \supset D_2$ by a rotation through $\pi/4$ about the z axis followed by a rotation through $\beta = \cos^{-1}(1/\surd 3)$ about the new y axis. This amounts to shifting the z axis from the [001] direction to the [111] direction (Watanabe 1966). The groups C_3 and D_2 may be embedded in the tetrahedral group T in different ways, each giving rise to a different integrity basis. These different embeddings amount to different choices of axes and usually do no more than change the signs associated with the invariants of degree 3, 4 and 6 (cf Abragam and Bleaney 1970).

The rotation properties of the angular momentum kets $|JM\rangle$ of degree 3, 4 and 6 readily yield the integrity bases as

$$T\supset D_2:\quad |00\rangle,\ i[|32\rangle-|3-2\rangle],\ |40\rangle+\frac{\sqrt{70}}{14}[|44\rangle+|4-4\rangle],$$

$$\left((|62\rangle+|6-2\rangle)-\frac{\sqrt{55}}{11}(|66\rangle-|6-6\rangle)\right) \tag{29}$$

$$T\supset C_3:\quad |00\rangle,\ |30\rangle+\frac{\sqrt{10}}{5}(|33\rangle-|3-3\rangle),\ |40\rangle-\frac{\sqrt{70}}{7}(|43\rangle-|4-3\rangle)$$

$$i\left((|63\rangle+|6-3\rangle)+\frac{\sqrt{110}}{22}(|66\rangle-|6-6\rangle)\right) \tag{30}$$

where in (29) the z axis is in the [001] direction and in (30) the [111] direction.

The $J=6$ representation of SO_3 yields the identity representation Γ_1 of T twice and thus there are two sixth-order invariants for T. However, one sixth-order invariant can always be formed from the square of the third-order invariant of T. In detail we have for $T\supset D_2$ the additional sixth-order invariant:

$$T\supset D_2:\quad |60\rangle-\frac{\sqrt{14}}{2}(|64\rangle+|6-4\rangle) \tag{31}$$

and for $T\supset C_3$ the additional sixth-order invariant

$$T\supset C_3:\quad |60\rangle+\frac{\sqrt{210}}{24}(|63\rangle-|6-3\rangle)+\frac{\sqrt{231}}{24}(|66\rangle+|6-6\rangle). \tag{32}$$

The invariant operators have exactly the same form as in (29) to (32) once the correspondence (25) is used. The eigenvalues and degeneracies of these operators are invariant with respect to changes in the relative signs that occur upon rotation to another set of equivalent axes, however the associated eigenvectors may be quite different.

8. Integrity bases and invariant operators for the octahedral group

The octahedral group O is made up of the pure rotations of the octahedron and contains the tetrahedral group T and the dihedral group D_4 as important subgroups. The integrity basis for O involves invariant polynomials of degree 0, 4, 6 and 9 (Meyer 1954).

The fourth- and sixth-order invariants of T given in (29) and (31) and in (30) and (32) for $T\supset D_2$ and $T\supset C_3$ respectively are also invariants under O. The third- and sixth-order invariants of T given in (29) and (30) for $T\supset D_2$ and $T\supset C_3$ respectively, transform under O as the Γ_2 representation. Since $\Gamma_2\times\Gamma_2=\Gamma_1$ the products of these third- and sixth-order invariants for T must yield invariants under O. The $D^{(9)}$ representation of SO_3, upon restriction to O, yields the identity representation Γ_1 just once and hence the ninth-order invariant may be built up via the methods of § 4 either by a coupling of the third- and sixth-order invariants of T or by a coupling of the fourth- and sixth-order invariants of O. These lower-order invariants fix the unnormalized transformation coefficients required for the right-hand side of (20) or (21). The $1jm$ and $3jm$ symbols on the left-hand side of (21) can be absorbed in the normalization of the ninth-order invariant. Proceeding in this way we obtain the invariants associated with the integrity basis for the octahedral group:

$\mathrm{O}\supset\mathrm{T}\supset\mathrm{D}_2$:

$$|00\rangle,\ |40\rangle+\frac{\sqrt{70}}{14}(|44\rangle+|4-4\rangle),\ |60\rangle-\frac{\sqrt{14}}{2}(|64\rangle+|6-4\rangle),$$

$$\mathrm{i}\left((|94\rangle-|9-4\rangle)-\frac{\sqrt{119}}{7}(|98\rangle-|9-8\rangle)\right) \tag{33}$$

and

$\mathrm{O}\supset\mathrm{T}\supset\mathrm{C}_3$:

$$|00\rangle,\ |40\rangle-\frac{\sqrt{70}}{7}(|43\rangle-|4-3\rangle),$$

$$|60\rangle+\frac{\sqrt{210}}{24}(|63\rangle-|6-3\rangle)+\frac{\sqrt{231}}{24}(|66\rangle+|6-6\rangle),$$

$$\mathrm{i}\left((|93\rangle+|9-3\rangle)+\frac{\sqrt{26}}{26}(|96\rangle-|9-6\rangle)-2\frac{\sqrt{663}}{221}(|99\rangle+|9-9\rangle)\right). \tag{34}$$

9. Integrity bases and invariant operators for the icosahedral group

The icosahedral group I is made up of the pure rotations of the icosahedron and is a non-crystallographic group. Nevertheless the icosahedral group finds important applications as an exact symmetry group for certain polyborane molecules (Muetterties and Knoth 1968) and as an approximate symmetry group for the rare earth double nitrates (Judd 1957, McLellan 1961, Tinsley 1963 and Devine 1967).

The integrity basis for I involves invariant polynomials of degree 0, 6, 10 and 15 (Meyer 1954). The z axis of the icosahedron may be chosen in many different ways (Cohen 1958). Choosing the z axis as a 5-fold axis corresponds to the group–subgroup scheme $\mathrm{I}\supset\mathrm{D}_5$. The choice of the z axis as a 2-fold or 3-fold axis corresponds to the group–subgroup schemes $\mathrm{I}\supset\mathrm{D}_2$ and $\mathrm{I}\supset\mathrm{C}_3$ respectively. Furthermore, the tetrahedral group occurs as a physically important subgroup (Devine 1967) giving rise to the group–subgroup chains $\mathrm{I}\supset\mathrm{T}\supset\mathrm{D}_2$ and $\mathrm{I}\supset\mathrm{T}\supset\mathrm{C}_3$.

It suffices to construct the sixth-order invariants as the tenth- and fifteenth-order invariants can then be constructed via the building-up principle. The sixth-order icosahedral invariants must involve linear combinations of the sixth-order invariants associated with the relevant subgroups. Thus we have for

$$\mathrm{I}\supset\mathrm{D}_5:\quad |60\rangle+\mathrm{i}x(|65\rangle+|6-5\rangle) \tag{35}$$

$\mathrm{I} \supset \mathrm{T} \supset \mathrm{D}_2$:

$$|60\rangle - \frac{\sqrt{14}}{2}(|64\rangle + |6-4\rangle) + y\left((|62\rangle + |6-2\rangle) - \frac{\sqrt{55}}{11}(|66\rangle + |6-6\rangle)\right) \tag{36}$$

$\mathrm{I} \supset \mathrm{T} \supset \mathrm{C}_3$:

$$|60\rangle + \frac{\sqrt{210}}{24}(|63\rangle - |6-3\rangle) + \frac{\sqrt{231}}{24}(|66\rangle + |6-6\rangle)$$

$$+ \mathrm{i}z\left((|63\rangle + |6-3\rangle) - \frac{\sqrt{110}}{22}(|66\rangle - |6-6\rangle)\right). \tag{37}$$

The numbers x, y, z remain to be determined. These numbers can be determined by demanding that the relevant linear combination remains invariant under any rotation that belongs to I but not to the relevant subgroups of I. The phases associated with these numbers will depend on the directions of the x and y axes relative to the icosahedron (Judd 1957, Boyle and Ozgo 1973, Boyle and Schäffer 1974). Of course this ambiguity of sign has no physical consequences provided the choice is made and then applied consistently throughout all practical calculations. Mixing of phase conventions is not permissible.

An alternative and much simpler approach for determining the relevant linear combinations is to diagonalize the operator eigenvalents for (35), (36) and (37) for the basis states $|3M\rangle$ and demand that the numbers x, y, or z be chosen so as to yield just two distinct eigenvalues one of degeneracy three and one of degeneracy four in accord with the branching rule $D^{(3)} \rightarrow U + V$ for $SO_3 \rightarrow \mathrm{I}$ (Griffith 1961). For example in the case of (35) we find the three 2-fold degenerate eigenvalues

$$-\frac{75\sqrt{231}}{54} \pm 15\left(\frac{21}{44} + 18x^2\right)^{1/2}, \frac{225\sqrt{231}}{77}$$

and the singly degenerate eigenvalue

$$-300\sqrt{231}/77.$$

There are two ways of combining these to obtain icosahedral degeneracy. These yield

$$x = \pm\sqrt{77}/11. \tag{38}$$

In an exactly similar manner we find that

$$y = \pm\sqrt{330}/22 \tag{39}$$

and

$$z = \pm 3\sqrt{14}/8. \tag{40}$$

The construction of the tenth- and fifteenth-order invariants from the sixth-order invariants is a straightforward application of the building-up principle. The tenth-order invariant is first formed from the coupled product of the sixth-order invariant with itself. The fifteenth-order invariant then follows from a coupling of the tenth- and sixth-order invariants. Here we give just the result for the tenth-order invariant for $\mathrm{I} \supset \mathrm{D}_5$

$$|10, 0\rangle \mp \mathrm{i}\frac{\sqrt{429}}{13}(|10, 5\rangle + |10, -5\rangle) - \frac{\sqrt{46189}}{247}(|10, 10\rangle + |10, -10\rangle). \qquad (41)$$

In these latter calculations the extensive tabulation of $3jm$ symbols by Bryant (1960) is most useful.

10. Application to the state labelling problem

The invariant operators derived from the integrity basis for $SO_3 \supset G$, where G is a finite rotation group, allow us to form complete sets of commuting operators which yield a solution of the state labelling problem with orthonormal eigenfunctions. Just two operators are required to form the set of commuting operators. It is natural to choose $\boldsymbol{J}^2$ as one member of the set. The second member of the set may be taken as any one of the remaining invariant operators, say $X_G^{(J)}$ transforming as the $D^{(J)}$ irreducible representation (irrep) of SO_3 or any suitable polynomial, say X_G, in $\boldsymbol{J}^2$ and the various $X_G^{(J)}$ associated with the subgroup chain of interest. The actual choice of X_G will depend on physical and computational considerations and must be such that the branching multiplicities associated with $SO_3 \to G$ are fully resolved. Thus for $SO_3 \supset D_2$ the choice of $X_{D_2}^{(3)}$ would be unsuitable as $X_{D_2}^{(3)}$ is also an invariant of the tetrahedral group T. If X is chosen as a real symmetric operator complex conjugate irreps of G will be undistinguished.

Eigenfunctions that simultaneously diagonalize the set of commuting operators $\{\boldsymbol{J}^2, X_G\}$ may be found by diagonalizing X_G in an $SO_3 \supset SO_2$ angular momentum basis $|JM\rangle$. Clearly to each $\{\boldsymbol{J}^2, X_G\}$ there will correspond a unique set of basis functions

$$|J\lambda\Gamma\gamma\rangle = \sum_M |JM\rangle\langle JM|J\lambda\Gamma\gamma\rangle \qquad (42)$$

where λ is an eigenvalue of X_G that serves to distinguish repetitions of the Γ irrep of G. In practice the γ labels could be obtained from the finite subgroups of G. The coefficients $\langle JM|J\lambda\Gamma\gamma\rangle$ are transformation coefficients that take us from the $SO_3 \supset SO_2$ basis to the $SO_3 \supset G$ basis.

Let us consider the reduction of the $D^{(2)}$ irrep of SO_3 under $SO_3 \to D_2$ where (Koster *et al* 1963)

$$D^{(2)} \to 2\Gamma_1 + \Gamma_2 + \Gamma_3 + \Gamma_4 \qquad (43)$$

and we choose to simultaneously diagonalize the set of commuting operators $\{J^2, X_{D_2}^{(2)}\}$ where

$$X_{D_2}^{(2)} = T_2^{(2)} + T_{-2}^{(2)} = \tfrac{1}{2}(J_+^2 + J_-^2). \qquad (44)$$

If $X_{D_2}^{(2)}$ is diagonalized in a JM basis with $J = 2$ we obtain the eigenvalues and eigenvectors shown in table 1. The transformation properties of the eigenvectors are readily deduced from standard projection operator techniques. We note here the two

Table 1. Eigenvalues and eigenvectors of $X^{(2)}_{D_2}$ in an angular momentum basis for $J=2$.

Eigenvalue	Eigenvector	Γ_i
0	$\|22\rangle_-$	Γ_3
3	$\|21\rangle_+$	Γ_2
-3	$\|21\rangle_-$	Γ_4
$2\sqrt{3}$	$(\|22\rangle_+ + \|20\rangle)/\sqrt{2}$	Γ_1
$-2\sqrt{3}$	$(\|22\rangle_+ - \|20\rangle)/\sqrt{2}$	Γ_1

Γ_1 irreps are distinguished, one is associated with the $\lambda = +2\sqrt{3}$ eigenvalue of $X^{(2)}_{D_2}$ and the other with $\lambda = -2\sqrt{3}$. We make frequent use of the abbreviation

$$|JM\rangle_\pm = \frac{1}{\sqrt{2}}(|JM\rangle \pm |J-M\rangle). \tag{45}$$

The basis functions obtained in table 1 are closely related to those of the asymmetrical top which arise when the operator (Patera and Winternitz 1973)

$$\begin{aligned} E &= 4(L_x^2 + rL_y^2) \qquad 0<r<1 \\ &= 2(1-r)X^{(2)}_{D_2} + 2(J^2 - J_z^2)(r+1) \end{aligned} \tag{46}$$

is diagonalized in the $|JM\rangle$ basis.

The reduction of $SO_3 \to T \to D_2$ for the $D^{(6)}$ irrep of SO_3 provides an interesting example of the labelling problem. We consider the two sets of commuting operators $\{\boldsymbol{J}^2, X^{(3)}_T\}$ and $\{\boldsymbol{J}^2, X^{(4)}_T\}$ where $X^{(3)}_T$ and $X^{(4)}_T$ are the rank 3 and 4 operators derived from (29). Under $SO_3 \to T$ we have

$$D^{(6)} \to 2\Gamma_1 + \Gamma_2 + \Gamma_3 + 3\Gamma_4. \tag{47}$$

Diagonalization of $X^{(3)}_T$ for the $|JM\rangle$ states where $J=6$ yields the eigenvalues

$$\lambda = \pm 6\sqrt{35}\,(1),\ \pm\frac{\sqrt{330}}{11}\,(1),\ \pm\frac{12\sqrt{935}}{11}\,(3),\ 0(3) \tag{48}$$

while $X^{(4)}_T$ yields the eigenvalues $12\lambda\sqrt{70}/7$ with

$$\lambda = 66(1),\ -126(1),\ 114(2),\ -96(3),\ 20 \pm 4\sqrt{421}\,(3) \tag{49}$$

where the eigenvalue degeneracies are given in brackets.

The eigenvalues associated with $X^{(3)}_T$ completely distinguish all the irreps of T contained in (47). The associated eigenvectors are given in table 2. We note that the diagonalization of $X^{(3)}_T$ yields a complex angular momentum basis and the eigenvalues λ of $X^{(3)}_T$ completes the labelling of the states. The eigenvalues associated with the complex conjugate irreps Γ_2 and Γ_3 of T differ in sign.

Diagonalization of $X^{(4)}_T$ yields a real angular momentum basis and the eigenvalues associated with Γ_2 and Γ_3 are identical as expected for a real basis. The eigenvalues of $X^{(4)}_T$, unlike those found for $X^{(3)}_T$, are not all pure irrational. This results in the associated eigenvectors assuming a rather complicated form. The bases obtained from the two pairs of commuting operators $\{\boldsymbol{J}^2, X^{(3)}_T\}$ and $\{\boldsymbol{J}^2, X^{(4)}_T\}$ are quite different. Either set of operators would yield an adequate set of labelled basis functions.

Table 2. Eigenvectors that simultaneously diagonalize $\{\boldsymbol{J}^2, X_{\mathrm{T}}^{(3)}\}$.

λ	Eigenvector in JM basis	Γ_i
0	$\left\{\begin{array}{l} \frac{1}{\sqrt{136}}(9\|66\rangle_- + \sqrt{55}\|62\rangle_-) \\ \frac{1}{\sqrt{17}}(\sqrt{6}\|65\rangle + \sqrt{11}\|61\rangle) \\ \frac{1}{\sqrt{17}}(\sqrt{6}\|6-5\rangle + \sqrt{11}\|6-1\rangle) \end{array}\right\}$	Γ_4
$\pm 12\frac{85}{\sqrt{11}}$	$\left\{\begin{array}{l} \frac{1}{\sqrt{272}}(-\sqrt{55}\|66\rangle_- \pm \mathrm{i}\sqrt{136}\|64\rangle_- + 9\|62\rangle_-) \\ \frac{1}{\sqrt{34}}(-\sqrt{11}\|65\rangle \pm \mathrm{i}\sqrt{17}\|63\rangle + \sqrt{6}\|61\rangle) \\ \frac{1}{\sqrt{34}}(-\sqrt{11}\|6-5\rangle \mp \mathrm{i}\sqrt{17}\|6-3\rangle + \sqrt{6}\|6-1\rangle) \end{array}\right\}$	Γ_4
$\pm\frac{30}{\sqrt{11}}$	$\left\{\frac{1}{8}(\mp \mathrm{i}\sqrt{22}\|66\rangle_+ + 2\|64\rangle_+ \pm \mathrm{i}\sqrt{10}\|62\rangle_+ + 2\sqrt{7}\|60\rangle)\right.$	$\left\{\begin{array}{l}\Gamma_2 \\ \Gamma_3\end{array}\right.$
$\pm 6\sqrt{35}$	$\left\{\frac{1}{8}(\mp \mathrm{i}\sqrt{10}\|66\rangle_+ - 2\sqrt{7}\|64\rangle_+ \pm \mathrm{i}\sqrt{22}\|62\rangle_+ + 2\|60\rangle)\right\}$	Γ_1

The study of the spectrum of the invariant operators and their associated bases deserves further study. We have indicated the relevance of one particular basis to the asymmetrical top and there are undoubtedly other important applications of other bases.

11. Symmetrization of the Gel'fand states

The Gel'fand states that arise in the canonical subgroup basis $\mathrm{U}_N \supset \mathrm{U}_{N-1} \supset \ldots \supset \mathrm{U}_1$ have been studied by many investigators (cf Louck 1970). More recently interest has been shown in the use of Gel'fand states in atomic (Patera 1972, Harter 1973, Drake *et al* 1975) and molecular (Paldus 1974, 1975) physics. These applications have all sought to capitalize on the existence of simple algorithms for constructing basis states and computing matrix elements.

In many physical problems there exists exact, or approximate invariance with respect to certain groups that is not apparent in the canonical formulation of the problems. Thus in many cases it is desirable to transform the canonical basis into some physically relevant non-canonical basis. This requires the symmetry adaption of the Gel'fand states. One solution to the problem of symmetry adaption is to demand that the Gel'fand states diagonalize a complete set of commuting operators associated with the non-canonical group structure. We sketch such a method.

The generators E_{ij} $(i, j = 1, 2, \ldots, N)$ of U_N satisfy the commutation relations

$$[E_{ij}, E_{kl}] = \delta_{jk}E_{il} - \delta_{il}E_{kj}. \tag{50}$$

The generators of the non-canonical angular momentum subgroup SO_3 may be expressed in terms of the generators of U_N by writing (Patera 1972)

$$\begin{aligned} J_+ &= \frac{1}{\sqrt{2}} \sum_{k=1}^{N-1} [k(N-k)]^{1/2} E_{k,k+1} \\ J_- &= \frac{1}{\sqrt{2}} \sum_{k=1}^{N-1} [k(N-k)]^{1/2} E_{k+1,k} \\ J_z &= \frac{1}{2} \sum_{k=1}^{N-1} k(N-k)(E_{k,k} - E_{k+1,k+1}). \end{aligned} \tag{51}$$

The Casimir invariant $\boldsymbol{J}^2$ of SO_3 can be expressed in terms of a quadratic in the generators of U_N via (51) and diagonalized by the Gel'fand states that have well defined transformation properties under SO_3. The SO_3 tensor operators $T_q^{(k)}$ may be realized as polynomials in $J_\pm$ and J_z via § 3 and thence as polynomials in the generators of U_N via (51). As a result every invariant operator X_G associated with a subgroup G of SO_3 may be realized as a polynomial in the generators of U_N. Diagonalization of the operator X_G will then yield linear combinations of the Gel'fand basis states that have well defined transformation properties with respect to both SO_3 and G.

The resulting eigenfunctions will be simultaneous eigenfunctions of $\{\boldsymbol{J}^2, X_G\}$ and may be designated by $|\alpha J\lambda\Gamma\gamma\rangle$ where α is a label introduced to distinguish repeated SO_3 irreps, J is the appropriate irrep of SO_3, λ the associated eigenvalue of X_G with Γ being an appropriate irrep of G and γ labelling the components of Γ. The labels α could come from invariant operators associated with the integrity basis for $U_N \supset SO_3$ while the γ labels could be replaced by those of a subgroup of G.

12. Relationship to coupling and transformation coefficients

The diagonalization of one of the operators X_G in the canonical $SO_3 \supset SO_2$ angular momentum $|JM\rangle$ basis yields a set of eigenvalues $[\lambda]$ that may be used to complete the labelling of the basis states for the non-canonical $SO_3 \supset G$ scheme. A typical non-canonical basis state that simultaneously diagonalizes $\boldsymbol{J}^2$ and X_G may be represented by the ket vector $|J\lambda\Gamma\gamma\rangle$ where λ is an eigenvalue of X_G associated with the irrep Γ of G and λ labels the components of Γ.

Th canonical $|JM\rangle$ basis is related by a unitary transformation to the non-canonical $|J\lambda\Gamma\gamma\rangle$ basis such that

$$|J\lambda\Gamma\gamma\rangle = \sum_M |JM\rangle\langle JM|J\lambda\Gamma\gamma\rangle \tag{52}$$

and

$$|JM\rangle = \sum_{\lambda\Gamma\gamma} |J\lambda\Gamma\gamma\rangle\langle J\lambda\Gamma\gamma|JM\rangle. \tag{53}$$

The coefficients of the expansion, $\langle JM|J\lambda\Gamma\gamma\rangle$, are the transformation coefficients that transform one basis into another (cf Butler 1975). Here these coefficients are in essence the elements of the unitary matrix that diagonalizes the operator X_G in the $|JM\rangle$ basis.

In practice the transformation coefficients are seldom amenable to an analytic formulation and must either be calculated recursively or obtained by diagonalization of suitable operators. In most cases it is difficult to avoid numerical calculation. The inherent difficulties in calculating transformation coefficients are readily seen in the case of the asymmetrical top (Patera and Winternitz 1973). Here the transformation coefficients involve the transformation from the canonical $SO_3 \supset SO_2$ basis to the non-canonical $SO_3 \supset D_2$ basis and even for angular momenta $J=2$ it is no longer possible to generally express all of the relevant transformation coefficients as pure rational or pure irrational numbers.

The transformation coefficients can be related to the coupling coefficients by considering the coupling of two kets in the non-canonical basis

$$|J_i\lambda_i\Gamma_i\gamma_i\rangle|J_j\lambda_j\Gamma_j\gamma_j\rangle = \sum_{\lambda\Gamma\gamma} |J\lambda\Gamma\gamma\rangle\langle J\lambda\Gamma\gamma|J_i\lambda_i\Gamma_i\gamma_i;\, J_j\lambda_j\Gamma_j\gamma_j\rangle. \tag{54}$$

The coupling coefficient can be factorized using Racahs' lemma (Racah 1949) and the kets on both sides expanded into the canonical basis using transformation coefficients. The properties of coupling coefficients (Butler 1975) may then be used to finally yield the relations.

$$\sum_{M_i,M_j} \langle JM|J_iM_i;\, J_jM_j\rangle\langle J_iM_i|J_i\lambda_i\Gamma_i\gamma_i\rangle\langle J_jM_j|J_j\lambda_j\Gamma_j\gamma_j\rangle$$

$$= \sum_{\lambda\Gamma\gamma\alpha} \langle JM|J\lambda\Gamma\gamma\rangle\langle J\lambda\Gamma\alpha|J_i\lambda_i\Gamma_i;\, J_j\lambda_j\Gamma_j\rangle\langle\alpha\Gamma\gamma|\Gamma_i\gamma_i;\, \Gamma_j\gamma_j\rangle. \tag{55}$$

This expression involves coupling and transformation coefficients. A restricted form of the above equation has been used by Golding in the calculation of coupling coefficients for the octahedral (Golding 1971) and icosahedral (Golding 1973) group.

It is important to note that (55) involves not only branching multiplicities λ but also product multiplicities α. These latter multiplicities arise in the application of the Racah factorization lemma to the coupling coefficient in (54). Application of the orthogonality property of coupling coefficients in (55) leads to the result (cf König and Kremer 1973, Harnung 1973)

$$\sum_{M,M_i,M_j} \langle J\lambda\Gamma\gamma|JM\rangle\langle JM|J_iM_i;\, J_jM_j\rangle\langle J_iM_i|J_i\lambda_i\Gamma_i\gamma_i\rangle\langle J_jM_j|J_j\lambda_j\Gamma_j\gamma_j\rangle$$

$$= \sum_{\alpha} \langle J\lambda\Gamma\alpha|J_i\lambda_i\Gamma_i;\, J_j\lambda_j\Gamma_j\rangle\langle\alpha\Gamma\gamma|\Gamma_i\gamma_i;\, \Gamma_j\gamma_j\rangle. \tag{56}$$

The two multiplicity problems are now clearly separated. The operators X_G give a systematic resolution of the branching multiplicities but not of the product multiplicities which must be independently considered. The angular momentum coupling coefficients on the left-hand side of (56) are known and the associated transformation coefficients follow from diagonalization of X_G in a $|JM\rangle$ basis. Thus the systematic resolution of the branching multiplicities leads to a complete determination of the left-hand side of (56). Hence the right-hand side of (56) is completely determined apart from the resolution of the product multiplicities. Clearly we have here a method of computing coupling coefficients. Different resolutions of the branching multiplicity result in different coupling coefficients. The actual choice of resolution must be decided on physical or computational considerations. It is apparent that some resolutions will lead to coupling coefficients of greater complexity than others as seen in the case of the asymmetrical top.

13. Extension to other groups

So far our attention has been restricted to the pure rotation subgroups of SO_3 and we exploited the close similarity between the transformation properties of states and tensor operators under pure rotations. Thus our results cover only eleven of the thirty-two crystallographic point groups. The remaining point groups involve inversion and reflections as well as pure finite rotations. We note reflections may be resolved into the product of a pure rotation followed by an inversion. Ten of the remaining point groups are isomorphic to pure rotation groups and the others can all be written as a direct product of a pure rotation group with the inversion group C_i.

The angular momentum states are not necessarily invariant with respect to inversions since

$$I|LM\rangle = (-1)^L|LM\rangle. \tag{57}$$

The angular momentum operators $J_\pm$, J_z all commute with I and hence the tensor operators used here are invariant with respect to inversions. This means that a group G' isomorphic to a given pure rotation subgroup G have the same invariant labelling operator X_G. The linear combinations of $|JM\rangle$ states that simultaneously diagonalize $\{\boldsymbol{J}^2, X_G\}$ will be the same for both groups but their transformation properties under the two groups may be different. The basis functions that are even with respect to inversion have the same transformation properties under G and G'. The odd basis functions will have the same transformation properties under G as the even basis functions. Under G' the odd and even basis functions will have different transformation properties and hence may be associated with different irreps of G'.

The remaining direct product groups $G \times C_i$ can be handled in a similar manner by enlarging the set of commuting operators to $\{\boldsymbol{J}^2, I, X_G\}$.

14. Conclusions

The introduction of integrity bases and the subsequent development of invariant operators for a non-canonical group–subgroup chain provides a systematic method for constructing complete sets of commuting operators. The eigenfunctions that simultaneously diagonalize a given set yield a fully labelled orthonormal basis for the representations associated with the group–subgroup chain. This provides a systematic and complete resolution of the branching multiplicity. It is important to note that the resolution obtained depends on the embeddings of the subgroups in the group chain and on the particular choice of polynomial invariant X_G.

We note that both product and branching multiplicities occur in coupling coefficients whereas the recoupling coefficients contain only product multiplicities. This would seem to add emphasis to the desirability of first calculating recoupling coefficients from first principles making an essentially ad hoc separation of the product multiplicities which are usually of no physical significance and then computing the coupling coefficients choosing the branching multiplicity resolution in the physically, or computationally, most appropriate manner (cf Butler and Wybourne 1976b).

It would seem to be imperative in preparing tables of coupling coefficients to specify the relevant group embeddings, the product multiplicity resolution and the choice of branching multiplicity resolution very carefully. It is possible for identical group chains to be associated with quite different sets of coupling coefficients.

The transformation coefficients involve only the branching multiplicity resolution and again this needs to be clearly specified in their tabulation.

The methods we have outlined for the special case of the finite subgroups of SO_3 can be extended to other groups and emphasize the central importance of coupling coefficients.

The construction of complete sets of polynomial invariants for group chains is likely to receive considerable application in spectral distribution methods where the moments $\langle H^p \rangle^{[\lambda]}$ of a Hamiltonian H are averaged over the states of a given irrep $[\lambda]$ of a group G (cf Hecht 1973). In these cases only the scalar parts of H^p survive and hence the moments can be expressed in terms of polynomial invariants. Specific applications to nuclear problems have been outlined by Quesne (1976, private communication) while the method of moments has been applied to the Jahn–Teller effect by Wagner (1970) but without reference to polynomial invariants.

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