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MONOMIAL REPRESENTATIONS OF OCTAHEDRAL GROUP SEQUENCES

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In a recent work A. Ceulemans and D. Beyens[1] show that monomial representations give rise to two interesting properties of the corresponding Clebsch-Gordan series: in the Kronecker product there is a natural separation of the repeated representations and, all the coupling coefficients are equal in absolute value.

In this note we want to show that some of the sequence -adapted irreducible representations (irreps) of the octahedral point group **O** can also be expressed in terms of monomial matrices. (We think that it can be possible an extension of this to many other solvable finite groups).

In order to study the irreps adapted in symmetry to the sequences of the octahedral group, it is convenient to define a set of generators of **O** which will allow us to determine the sequences in a simple direct way. Since **O** have the composition series $\mathbf{O} \triangleright \mathbf{T} \triangleright \mathbf{D}_2^* \triangleright \mathbf{C}_2 \triangleright \mathbf{C}_1$, we know that it is a solvable group[2] and that all its irreps are equivalent to monomial matrices[3]. From the factor groups $\mathbf{O}/\mathbf{T}$, $\mathbf{T}/\mathbf{D}_2^*$ and $\mathbf{D}_2^*/\mathbf{C}_2$, we can define four generators $g_i \in \mathbf{O}$ such that $g_1 \in \{8C_3\}$, $g_2 \in \{6C_2'\}$ and $(g_3, g_4) \in \{3C_2\}$, where the sets between curly brackets are classes of **O**.

Using the induced representation theorem[4] we construct the irreps of our generators $g_i \in \mathbf{O}$ from the irreps of the subgroups of **O**. Taking the irrep A of $\mathbf{D}_2^*$ we induce the one-dimensional irreps A, E_1, E_2 of **T** and, from one of the irreps B_i (i=1,2,3) of $\mathbf{D}_2^*$, we calculate the three-dimensional irrep T of **T** group.

Since T is induced from a one-dimensional irrep, it will be given in monomial form[5]. As the kernel of the ground representation of **T** by $\mathbf{D}_2^*$ is $\mathbf{D}_2^*$, the irrep T is symmetry adapted to the sequence $\mathbf{T} \triangleright \mathbf{D}_2^*$ [6]. The induction of the irrep E of $\mathbf{O}$ from the irreps of the group $\mathbf{T}$ is performed in the same way as that of T of $\mathbf{T}$ from $\mathbf{D}_2^*$.

The problem whether or not the irreps T_1 and T_2 of $\mathbf{O}$ group can be induced from a given T of $\mathbf{T}$ preserving the monomial form, can be solved using a simple transformation.

Let θ be an homomorphism such that we induce from T of $\mathbf{T}$ a representation which contains T_1 and T_2 of $\mathbf{O}$:

$$\theta : g \to \begin{pmatrix} T(g) & 0 \\ 0 & T(g_2 g\, g_2) \end{pmatrix}$$

$$\theta : g_2 g \to \begin{pmatrix} 0 & \mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix} \begin{pmatrix} T(g) & 0 \\ 0 & T(g_2 g\, g_2) \end{pmatrix} ,$$

where $g \in \mathbf{T}$ and $\mathbb{1}$ is the identity matrix of the irrep T of $\mathbf{T}$

Then, if

$$A = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} , \text{ using a transformation } \mathbf{U} = \frac{1}{\sqrt{2}} \begin{pmatrix} \mathbb{1} & \mathbf{A} \\ \mathbb{1} & \mathbf{A} \end{pmatrix} ,$$

we have an homomorphism θ' such that

$$\theta' : g \to \begin{pmatrix} T(g) & 0 \\ 0 & T(g) \end{pmatrix} , \text{ and } \theta' : g_2 g \to \begin{pmatrix} \mathbf{A} & 0 \\ 0 & -\mathbf{A} \end{pmatrix} \begin{pmatrix} T(g) & 0 \\ 0 & T(g) \end{pmatrix} .$$

These are the irreps T_1 and T_2 which, together with E of $\mathbf{O}$ are given in Table I.

The behavior of the basis kets belonging to monomial irreps of the octahedral group is given in Table I of reference (1). Clearly, the irreps constructed using that table are adapted in symmetry to the sequence $\mathbf{O} \triangleright \mathbf{T} \triangleright \mathbf{D}_2^* \triangleright \mathbf{C}_2$, and coincide with those given in Table I.

In order to extend these results to the other sequences of the octahedral group we first use a particular realization of the generators g_i. Let us take $g_1 = C_3^{xyz}$, $g_2 = C_2^{x\bar{y}}$, $g_3 = C_2^x$, $g_4 = C_2^z$. Table II shows the subgroups of $\mathbf{O}$ given in terms of these generators. It is interesting to note that any other realization of the generators can be obtained from the given one, just by conjugation under the elements of $\mathbf{O}$ group[7]. This is the reason why we include in Table II the normalizer groups $N(\mathbf{G}_i) = \{g \in \mathbf{O} \mid g\,\mathbf{G}_i\, g^{-1} = \mathbf{G}_i\}$ with $\mathbf{G}_i \leq \mathbf{O}$.

As a second step we use Table II to determine all possible sequences of $\mathbf{O}$. The result is given in Figure I where, for simplicity, the sequences are interrupted in their maximal abelian subgroups. This interruption does not introduce any indetermination in the corresponding symmetry-adapted irreps since a representation of an abelian group must be given by diagonal matrices and, therefore, it is always automatically adapted to any sequence of subgroups.

Finally, the irreps adapted to the sequences given in Figure I are obtained by unitary transformations applied to the generators matrices given in Table I[8]. The results are shown in Table III, where we give the irreps of the generators of $\mathbf{O}$ which can be written in monomial form, and which are adapted to the sequences of the octahedral group.

By inspection of Table III we see that the irreps T_1

and T_2 of **O** group have an identical behavior with respect to the sequences. This is due to the relation that exists between them: $A_2 \times T_1 = T_2$, which allows the calculation of one from the other. Thus, when one of them is given in monomial form, the other one also is.

It must be remarked that the results of Table III are valid also for the odd and even irreps of $\mathbf{O}_h$, adapted to the sequences of subgroups which are the direct product of $\mathbf{C}_i$ with those subgroups of **O** shown in Table II. Moreover, through an automorphism of $\mathbf{O}_h$ that maps the group onto itself it is possible to show that the irreps given in Table I are symmetry adapted also to the sequence $\mathbf{O}_h \triangleright \mathbf{T}_d \triangleright \mathbf{D}_{2d} \triangleright \mathbf{D}_2^*$.

REFERENCES

(1) A. Ceulemans and D. Deyens - Phys. Rev. A 27, 621 (1983).

(2) D.J.S. Robinson - "A course in the Theory of Groups". Graduate Texts in Math. 80. Springler Verlag, N.Y. (1982). P. 143.

(3) Reference (2), p. 237.

(4) S.L. Altmann, "Induced Representations in Crystals and Molecules". Ac. Press, London (1977). P. 138.

(5) Reference (2), P. 235.

(6) Reference (4), P. 193.

(7) The application of an element $\phi \in \mathrm{Aut}\,\mathbf{G}$ on the generators g_i of a finite group **G** will in general results in new generators g_i^{ϕ} which give isomorphic copies of **G**. Since **O** is isomorphic to $\mathbf{S}_4$, it only has inner automorphism.

(8) It is important to note that when the sequences in question contain a group that is not an invariant subgroup of the preceding one, we can not apply the induction method to obtain the symmetry-adapted irreps to the sequences.

Caption to the Tables

Table I: Irreducible representations for the generators $g_i \in \mathbf{O}$ $\omega = \exp\{2\pi i/3\}$.

Table II: Generators of the octahedral group and its non abelian subgroups.

Table III: Generators of $\mathbf{O}$ which admit monomial representations a dapted to the sequences.

Caption to the Figure

Figure I: The sequences of the octahedral group corresponding to our particular choice of the generators.

Table I

$\mathbb{O}$	$C_2^{\,x\bar{y}}$	$\mathbb{T}$	$C_3^{\,xyz}$	$\mathbb{D}_2^*$	$C_2^{\,x}$	$C_2^{\,z}$
E	$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$	E_2 E_1	$\begin{pmatrix} \omega^* & 0 \\ 0 & \omega \end{pmatrix}$	A A	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$
T_1 T_2	$\mp\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	T	$\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$	B_3 B_2 B_1	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$

Table II

$\mathbb{G}_i$	g_1	g_2	g_3	g_4	$N(\mathbb{G}_i)$
$\mathbb{O}$	1	1	1	1	$\mathbb{O}$
$\mathbb{T}$	1		1	1	$\mathbb{O}$
$\mathbb{D}_4$		1	1	1	$\mathbb{D}_4$
$\mathbb{D}_3$	1	1			$\mathbb{D}_3$
$\mathbb{D}_2^*$			1	1	$\mathbb{O}$
$\mathbb{D}_2$		1		1	$\mathbb{D}_4$

Table III

sequences / irreps	I	II,VI	III	IV,V
E	g_1, g_2, g_3, g_4	g_1, g_2, g_3, g_4	g_2, g_3, g_4	g_2, g_3, g_4
T_1, T_2	g_1, g_2, g_3, g_4	g_1, g_2	g_1, g_2, g_3, g_4	g_2, g_3, g_4

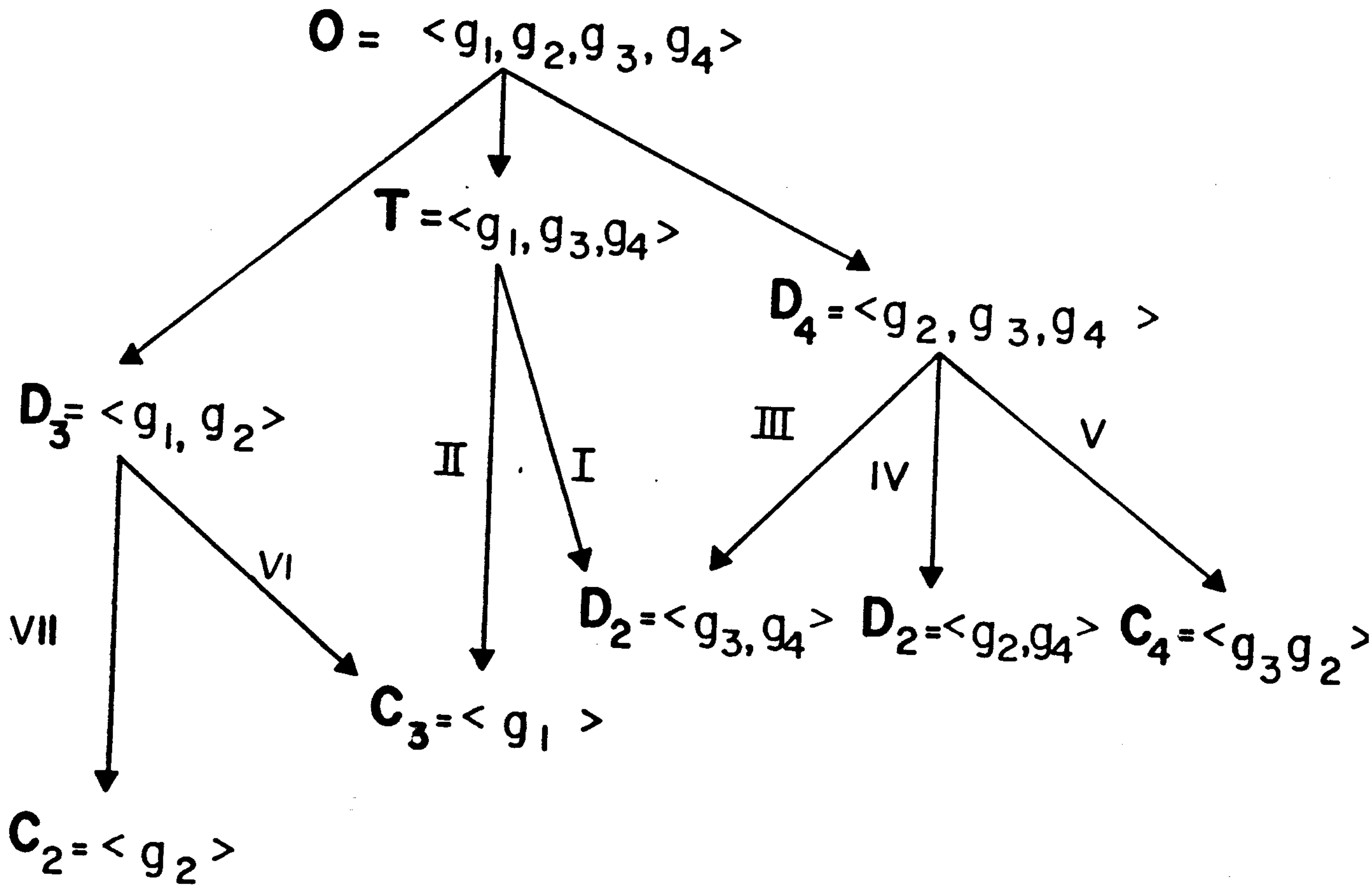
O = <g1, g2, g3, g4>
T = <g1, g3, g4>
D4 = <g2, g3, g4 >
D3 = <g1, g2>
II
I
III
IV
V
VI
VII
D2 = <g3, g4>
D2 = <g2, g4>
C4 = <g3 g2>
C3 = <g1 >
C2 = <g2 >

FIGURA I