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FINITE GROUPS LATTICES AND AUTOMORPHISMS

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A B S T R A C T

The present paper is part of a systematic labour to determine the symmetry adapted irreducible representations of the sequences of maximal subgroups of a given finite group. We prove that the elements of the group of automorphisms of a finite group allow the reduction of the number of chains for which it is necessary to calculate the irreducible representations. Moreover, if the outer automorphisms of a finite group have the property of interchange classes of conjugate elements, we show that it is also possible to reduce the number of irreducible representations to be calculated.

The method developed is applied explicitly to the maximal subgroups lattice of the dihedral group $D_{2\alpha}$ which is isomorphic to $C_{2\alpha,v}$ and $D_{2^{\alpha-1},d}$. We then discuss the application of the method to crystallographic point groups, as well as the use of automorphisms to establishing relations between the Clebsch-Gordan coefficients of a finite group.

1. INTRODUCTION

The investigation of chains involving continuous as well as finite groups has become very familiar to physicists and chemists during recent years. Group chains turn out to be particularly useful in the study of broken symmetry arising either via descent in symmetry or via spontaneous symmetry breaking. Moreover, the consideration of a group-subgroup chain throws light on the structural significance of the system under consideration and, if a suitable chain of groups is chosen, it leads to the elimination of the multiplicity problem thereby solving the question of labelling the basis states unambigously.

Suppose we have a set of sequences of subgroups of a finite group G with the property that each sequence is formed by maximal subgroups . Let Aut G be the group of automorphisms of G and let us define a *fundamental lattice* of a finite group as the one formed by all the sequences of maximal subgroups which are not related by the elements of Aut G . Therefore, given any other sequence of maximal subgroups, there always is, at least, one element $\varphi \in$ Aut G which allows the derivation of the given chain, from a sequence belonging to the fundamental lattice. Furthermore, the irreducible representation (irrep) adapted in symmetry to the given sequence is obtained by applying the same transformation to the irrep adapted to that chain of subgroups belonging to the fundamental lattice.

φ : phi
$\in$: belongs to

To achieve our objective we start in section 2 by giving the theory necessary to obtain the irreps adapted to any chain of a finite group G from those irreps adapted to the chains of the fundamental lattice of G .

The application of the method depends on the knowledge of Aut G and the complete lattice of maximal subgroups of G which, in turn, allows the determination of the fundamental lattice of maximal subgroups of G .

As an example of application we chose the set of dihedral groups D_{2^α} for several reasons. First , the dihedral groups are generated by two elements and, since 2^α is a co-prime number to any odd number, the group Aut D_{2^α} can be determined in a general form and decomposed into the product of three of its subgroups. This is shown in detail in section 3 .

The second reason is that the complete lattice of the group D_{2^α} can be exactly determined. This is done in section 4, where we also introduce a compact nomenclature for the sequences. The notation allows a direct determination of the generators of a maximal subgroup , just suppressing one of them , on the left of the set of generators which define the dihedral group and can also be used to label all the sequences of crystallographic point groups.

$G_1 \supset G_2$: G_2 is contained in G_1

Finally, it must be pointed out that the irreps adapted to the sequence $D_{2^\alpha} \supset C_{2^\alpha}$ can be deduced in a simple algebraic manner, making easy the presentation of the results .

In section 5 we find explicitly the irreps adapted to the sequences belonging to the fundamental lattice and to the complete lattice, in a way that applies to any crystallographic (or not) point group. In order to avoid some complexity in the tables given in that section, we restrict part of our calculation to the non-crystallographic point group D_8, which is isomorphic to C_{8v} and D_{4d} .

The method given in section 2 to find the irreps of a finite group is discussed in section 6 , in terms of convenient orderly steps of application, in particular, to crystallographic point groups.

In that section, we also analyze the role of the outer automorphisms which, besides establishing symmetry relations between the Clebsch-Gordan coefficients of the group, determine as well the isomorphisms between the subgroups of a group. If we take, for example, Tisza isomorphism $D_8 \simeq C_{8v} \simeq D_{4d}$, we easily see that it results from outer automorphisms of D_{8h} and, the isomorphism $T_d \simeq O$, comes from the unique outer automorphism of the group O_h .

$\simeq$ isomorphic to

Finally, in appendix I we demonstrate a theorem that reduces the number of irreps which necessarily must be computed by the induction method.

2. IRREPS CALCULATION FOR A LATTICE

A system of subgroups of a finite group G

1 unit element

$$G = G_0 \supset G_1 \supset G_2 \supset \ldots \supset G_k = \mathbb{1}$$

beginning with G itself and ending with the unit subgroup, is called a maximal subgroup sequence of G if $\forall$ $G_i \supset G_{i+1}$ it does not exist a group H such that $G_i \supset H \supset G_{i+1}$.

∀ for all

We say that two sequences of groups are different when they differ at least by one arbitrary group G_i.

An irrep of a finite group G, adapted in symmetry to one of its sequences is given through an homomorphism induced by $\Gamma_n^{(0)}$, defined such that(*)

$$\Gamma_n^{(0)} : g_\ell \equiv \Gamma_n^{(0)}(g_\ell) = A_{n,\ell}^{(0)} \qquad \forall\ g_\ell \in G .$$

n numbers not equivalent irreps of G , $A_{n,\ell}^{(0)}$ are unitary matrices, and

⊕ direct sum

$$\Gamma_n^{(i)}(g_\ell) = \bigoplus_{n'} \nu(n/n')\ \Gamma_{n'}^{(i+1)}(g_\ell) \quad ,$$

$$\forall\ g_\ell \in G_{i+1} \subset G_i \ , \ i = 0,1,\ldots,n-1 .$$

$\nu(n/n')$ is the frequency of $\Gamma_{n'}^{(i+1)}$ in $\Gamma_n^{(i)}$.

In particular, an irrep of an abelian group is adapted in symmetry to every one of its subgroups. Thus, an irrep can be adapted to more than one sequence of a lattice. In this work we interrupt the sequences which form a lattice in their maximal abelian subgroup. Therefore,

(*) All the irreps in this work are assumed to be unitary matrices.

there is one system of irreps for each sequence appearing in a lattice.

The lattice of maximal subgroups can be constructed through the mappings induced by the elements $\varphi \in \text{Aut } G$ which carry the original sequence to the image chain $G \supset G_1^{\varphi} \supset G_2^{\varphi} \supset \ldots \supset G_k^{\varphi}$. The set G_i^{φ} is a group of elements $\{\varphi : g_\ell\}$ $\forall\, g_\ell \in G_i$ $(i=1,2,\ldots,k)$. On the other hand, if we apply the same automorphism on the irrep adapted to a sequence belonging to the fundamental lattice, it generates an irrep adapted to the image chain $\Gamma_n^{\varphi}(g_\ell) = \Gamma_n(\varphi^{-1} : g_\ell)$. This is shown in figure 1 .

The question now is : among the automor - phisms $\varphi \in \text{Aut } G$, which of them give different resultant sequences ?

In order to see that, we first define a group

$$S_G(G_i) = \{\varphi \in \text{Aut } G \mid G_i^{\varphi} = G_i\} \; .$$

∩ intersection

Obviously,

$$S_G(G_i) = \text{Aut } G \cap \text{Aut } G_i \; ,$$

and it is a subgroup of Aut G .

Now, if we define another group,

$$_GS = \bigcap_{i=1}^{n} S_G(G_i) = \bigcap_{i=1}^{n} \text{Aut } G_i \; ,$$

which also is a subgroup of Aut G, every element $\varphi \in {}_GS$ will map a maximal subgroup sequence onto itself.

Writing Aut G in terms of the cosets of ${}_GS$ we have,

$$\mathrm{Aut}\ G = \bigoplus_{\eta=1}^{|\eta|} \varphi_\eta\ {}_G S \quad , \qquad (2.1)$$

where $|\eta| = |\mathrm{Aut}\ G| / |{}_G S|$.

We now proceed to prove that if φ_1 and φ_2 are two elements belonging to different cosets of ${}_G S$, the induced sequences $G \supset G_1^{\varphi_1} \supset \ldots \supset G_k^{\varphi_1}$ and $G \supset G_1^{\varphi_2} \supset \ldots \supset G_k^{\varphi_2}$ are always different. For this purpose we assume the contrary :

$$G_i^{\varphi_1} = G_i^{\varphi_2} \quad \forall \ i = 1,2,\ldots,k \ .$$

Since $\varphi_i \in \mathrm{Aut}\ G$ there exists φ_i^{-1} such that $(G_i^{\varphi_1})^{\varphi_2^{-1}} = G_i$. Hence, φ_1 and φ_2 must belong to the same coset of ${}_G S$, against the hypothesis.

Let us consider another important question : which is the subset of elements $\varphi \in {}_G S$ such that $\Gamma_n^\varphi \nsim \Gamma_n$, i.e. which elements of ${}_G S$ induce inequivalent irreps ? In order to see that, we define a group

φ not equivalent

$$K_S(\Gamma_n) = \{ \varphi \in {}_G S \mid \Gamma_n^\varphi \sim \Gamma_n \} \quad ,$$

~ equivalent

which is a subgroup of ${}_G S$. If we decompose the group ${}_G S$ into cosets of its subgroup $K_S(\Gamma_n)$, we have

$${}_G S = \bigoplus_{\gamma=1}^{|\gamma|} \varphi_\gamma \ K_S(\Gamma_n) \quad , \qquad (2.2)$$

where $|\gamma| = |{}_G S| / |K_S(\Gamma_n)|$.

We are going to prove that if φ_1 and φ_2 belong to different cosets of K_S , the irreps $\Gamma_n^{\varphi_1}$ and $\Gamma_n^{\varphi_2}$ are inequivalent. We assume the contrary : $\Gamma_n^{\varphi_1} \sim \Gamma_n^{\varphi_2}$.

If this is so, there is φ_2^{-1} such that $\Gamma_n^{\varphi_2^{-1}\varphi_1} \sim \Gamma_n$, i.e. φ_2 , φ_1 belong to the same coset of K_S, contrary to the hypothesis. Therefore, only elements of the same coset of K_S induce equivalent irreps.

We need now to show that $\forall\ \varphi \in \mathrm{Aut}\ G,\ \Gamma_n^{\varphi} \not\sim \Gamma_{n'}^{\varphi}$ $(n' \neq n)$. Assuming, on the contrary, that $\Gamma_n^{\varphi} \sim \Gamma_{n'}^{\varphi}$, there is a unitary transformation U such that

$$\Gamma_n^{\varphi}(g_\ell) = U\ \Gamma_{n'}^{\varphi}(g_\ell)\ U^{\dagger} \qquad \forall\ g_\ell \in G \ .$$

But, from $\Gamma_m^{\varphi}(g_\ell) = \Gamma_m(\varphi^{-1} : g_\ell = g_{\ell'})$, valid for every irrep of G, we directly obtain $\Gamma_n(g_{\ell'}) \sim \Gamma_{n'}(g_{\ell'})$, contradicting definition of n .

As we have seen in section 1, it is possible that the fundamental lattice may be formed by more than one sequence. In this case, it is convenient to define the isotropic group of the irreps,

$$K_A(\Gamma_n) = \{ \varphi \in \mathrm{Aut}\ G \mid \Gamma_n^{\varphi} \sim \Gamma_n \} \ ,$$

such that $K_S(\Gamma_n)$ is a subgroup of $K_A(\Gamma_n)$.

Writing ${}_G S^{\mu}$ and K_S^{μ} , the index μ indicating the different sequences which belong to the fundamental lattice, we have

$$K_S^{\mu}(\Gamma_n) = {}_G S^{\mu} \cap K_A(\Gamma_n) \ . \tag{2.3}$$

The task of determine the elements of $K_A(\Gamma_n)$ is simplified considerably by the fact that the group of inner automorphisms of G, Inn G, is a subgroup of $K_A(\Gamma_n)$ and it is isomorphic to the factor group G/Z(G), being Z(G) the center of G . Then, we only need to analyze the action of the elements of the factor group Aut G/ Inn G on the irreps of G .

3. GROUP OF AUTOMORPHISMS OF A DIHEDRAL GROUP $D_{2\alpha}$

Let $<\rho>$ and $<\varepsilon>$ be two groups generated by some arbitrary operations ρ and ε. Let n be any integer $n \geq 2$. If $\rho^n = \varepsilon^2 = \mathbb{1}$, $\varepsilon\rho = \rho^{-1}\varepsilon$ and $<\rho> \cap <\varepsilon> = \mathbb{1}$, ρ and ε are the generators of the group $D_n = <\rho,\varepsilon>$ with elements $\{\mathbb{1},\rho,\rho^2,\ldots,\rho^{n-1},\varepsilon,\rho\varepsilon,\rho^2\varepsilon,\ldots,\rho^{n-1}\varepsilon\}$.

It is clear that, associated with the definition of a dihedral group, we have the isomorphic groups given by

$$D_{2\alpha} = < C^z_{2\alpha}, C^x_2 > \quad ,$$

$$C_{2\alpha,v} = < C^z_{2\alpha}, IC^x_2 > \quad ,$$

$$D_{2\alpha-1,d} = < IC^z_{2\alpha}, IC^x_2 > \simeq < IC^z_{2\alpha}, C'_2 > \quad ,$$

where $C^{\vec{n}}_{\nu}$ is a symmetry operation by rotation in an angle $2\pi/\nu$ around the $\vec{n}$ axis and I is the inversion operation. Furthermore, the isomorphisms that relate these groups are outer automorphisms of the group $D_{2\alpha,h} = <C^z_{2\alpha}, C^x_2> \otimes <I>$ and it must be noted that $D_{2\alpha}$, $C_{2\alpha,v}$ and $D_{2\alpha-1,d}$ are maximal invariant subgroups of $D_{2\alpha,h}$.

$\otimes$ direct product

In order to determine the group of automorphisms of a dihedral group we use the property that the order $o(g)$ of an element g of a finite group G is preserved by the transformations of the group of its automorphisms .

This means that, if $o(g) = h$, then $o(\varphi:g) = h \ \forall \varphi \in \mathrm{Aut}\ G$. For $n = 2^{\alpha}$, $o(\rho^{2k+1}) = 2^{\alpha} \ \forall\ k = 0,1,2,\dots$. Then, for $\alpha > 2$ we have mappings such that :

$$\varphi : \rho^{2k+1} \to \rho^{2s(k)+1} ,$$

where $s(k)$ are integer numbers. Calling $s(0) = m$, we get

$$\varphi : \rho \to \rho^{2m+1} .$$

Then,
$$\varphi : \rho^{k} = (\varphi : \rho)^{k} \to \rho^{(2m+1)k} ,$$

with the fixed points $\mathbb{1}$ and $\rho^{2^{\alpha-1}}$. Now, since $o(\rho^{k}\varepsilon) = 2$ $\forall\ k$, we can define an element $\varphi(\lambda,\tau)$, that we write briefly (λ,τ) , such that it induces on the elements of the group $D_{2\alpha}$ the following mappings :

$$(\lambda,\tau) : \rho^{k} \to \rho^{\lambda k} \tag{3.1}$$

$$(\lambda,\tau) : \rho^{k'}\varepsilon \to \rho^{\lambda k'+\tau}\varepsilon ,$$

where k, k', λ and τ are integer positive numbers less than or equal to 2^{α}, and λ is an odd number.

The law of combination of the elements (λ,τ) is given by :

$$(\lambda_1,\tau_1)(\lambda_2,\tau_2) = (\lambda_1\lambda_2,\lambda_1\tau_2+\tau_1)\ Mod\ 2^{\alpha} . \tag{3.2}$$

The unit element of the set $\{(\lambda,\tau)\}$ is $(1,0)$ and the inverse of (λ,τ) is the element $(\lambda,\tau)^{-1} = (\lambda^{-1},-\lambda^{-1}\tau)$, with $\lambda\lambda^{-1} = 1\ Mod\ 2^{\alpha}$. Then, we conclude that the set of auto - morphisms (λ,τ) forms the group $\mathrm{Aut}\ D_{2\alpha}$.

Now we want to show that the group Aut $D_{2\alpha}$ can be written as a triplet product of some of its subgroups. In order to obtain such expression we use equation (3.2) and write an arbitrary element (λ,τ) in the following form :

$$(\lambda,\tau) = (1,1)^{\tau}(\lambda,0) = (\lambda,0)(1,1)^{\tau'}, \quad (3.3)$$

where τ' is such that $\lambda\tau' = \tau \; Mod \; 2^{\alpha}$.

Clearly, since

$$<(1,1)> \cap <(\lambda,0)> = (1,0) \quad ,$$

we are able to write

⊗ semidirect product

$$\text{Aut } D_{2\alpha} = <(1,1)> \otimes <(\lambda,0)> \quad , \quad (3.4)$$

where $<(\lambda,0)>$ is the abelian group of all the odd numbers less than 2^{α} under the operation of multiplication $Mod\; 2^{\alpha}$.

We prove now that it is always possible to generate the group $<(\lambda,0)>$ from the elements $(3,0)$ and $(2^{\alpha}-1,0)$ such that we can write

$$<(\lambda,0)> = <(3,0)> \otimes <(2^{\alpha}-1,0)> \quad , \quad \alpha \geq 3 \; . \quad (3.5)$$

By induction we get that, for $\alpha \geq 4$, $3^{2^{\alpha-3}} = (1 + 2^{\alpha-1}) \; Mod \; 2^{\alpha}$. Then, $3^{2^{\alpha-2}} = 1 \; Mod \; 2^{\alpha}$ for $\alpha \geq 3$. On the other hand, we must prove that $k = 2^{\alpha-2}$ is the less power for which the property $3^{k} = 1 \; Mod \; 2^{\alpha}$ holds. Suppose, on the contrary, that there exists $k < 2^{\alpha-3}$ with that property. Therefore, since k must be a divisor of $2^{\alpha-2}$, we can write $k = 2^{\beta}$ $(\beta < \alpha-3)$. But in this case, $(3^{2^{\beta}})^{\alpha-3-\beta} = (1 + 2^{\alpha-1}) \; Mod \; 2^{\alpha}$ for $\alpha-3-\beta>0$.

This relation shows that there is no $k < 2^{\alpha-3}$. Therefore, we can conclude that the $2^{\alpha-2}$ powers of $3 \; Mod \; 2^{\alpha}$ are distinct; moreover, they are the elements of the cyclic group $<(3,0)>$.

Using this result we make the coset expansion of $<(\lambda,0)>$ with respect to its normal subgroup $<(3,0)>$:

$$<(\lambda,0)> = <(3,0)> \oplus u <(3,0)> \quad . \qquad (3.6)$$

Since every abelian group can be expressed as a direct product of cyclic groups(1) it must exist an element u which belongs to $<(\lambda,0)>$ and is not contained in $<(3,0)>$ such that $u^2 = 1 \; Mod \; 2^{\alpha}$. It is easy to verify(2) that the four roots of this equation are : $u = 1, \; 2^{\alpha-1} - 1$, $2^{\alpha-1} + 1$ and $2^{\alpha} - 1$. We then choose the last root because it defines the element $(2^{\alpha}-1,0)$ which, in turn, induces the mappings $\rho^k \to \rho^{-k}$, $\rho^k\varepsilon \to \rho^{-k}\varepsilon$. This choice completes the proof of equation (3.5) .

Equation (3.4) can now be rewritten as

$$\text{Aut } D_{2\alpha} = <(1,1)> \oslash \{<(3,0)> \otimes <(2^{\alpha}-1,0)>\} \; , \quad \alpha \geq 3. \qquad (3.7)$$

Clearly, this equation remains true if $\alpha=2$, that gives the group D_4 ; but since $2^{\alpha}-1 = 3$, equation (3.7) becomes

$$\text{Aut } D_4 = <(1,1)> \oslash <(3,0)> \quad . \qquad (3.8)$$

(1) W.Ledermann, "Introduction to the theory of finite groups", p.142. Oliver and Boyd: Edinburg (1957).

(2) L.E.Dickson, "Introduction to the theory of numbers", p.14. Dover Publ.Inc. N.Y. (1957).

It must be noted that our result is not valid for $\alpha = 1$, since in this case we get the group D_2 which, being abelian, has Inn $D_2 = \mathbb{1}$. The outer automorphisms are given by the permutations of the elements ε, ρ and $\rho\varepsilon$. Thus, Aut D_2 is isomorphic to S_3, the symmetric group of degree 3.

We can also write the group of the inner automorphisms of $D_{2\alpha}$ as a semidirect product, using the following transformations :

$$\rho^{\tau}(\rho^{k}\varepsilon)\rho^{-\tau} = \rho^{k+2\tau}\varepsilon = (1,1)^{2\tau} : \rho^{k}\varepsilon \; ,$$

$$\rho^{\tau}\varepsilon(\rho^{k}\varepsilon)\rho^{\tau}\varepsilon = \rho^{-k+2\tau}\varepsilon = (1,1)^{2\tau}(2^{\alpha}-1,0) : \rho^{k}\varepsilon . \tag{3.9}$$

Then, for $\alpha \geq 2$ we have,

$$\text{Inn } D_{2\alpha} = \langle(1,2)\rangle \circledS \langle(2^{\alpha}-1,0)\rangle \; , \tag{3.10}$$

where $(1,2) = (1,1)^{2}$.

Finally, using equation (3.10) into (3.7) we obtain

$$\text{Aut } D_{2\alpha}/\text{Inn } D_{2\alpha} = \langle(3,0)\rangle \text{ Inn } D_{2\alpha} \oplus$$

$$(1,1) \langle(3,0)\rangle \text{ Inn } D_{2\alpha} \; . \tag{3.11}$$

This equation shows that the elements $(3^{\ell},0)$ and $(3^{\ell},1)$ with $0 < \ell \leq 2^{\alpha-2}$, are coset representatives of Inn $D_{2\alpha}$ in Aut$D_{2\alpha}$ for $\alpha \geq 2$.

4. THE LATTICE OF A DIHEDRAL GROUP $D_{2\alpha}$

In order to establish the sequences of the dihedral group $D_{2\alpha}$ we decompose the group into semidirect (direct) products of its subgroups, for $\alpha > 1$ $(\alpha = 1)$:

$$\begin{aligned} <\rho,\varepsilon> &= <\rho> \circledS <\varepsilon> \\ &= <\rho^2,\varepsilon> \circledS <\rho\varepsilon> \quad . \end{aligned} \tag{4.1}$$

This equation shows that $<\rho>$ and $<\rho^2,\varepsilon>$ are subgroups of $D_{2\alpha}$ of order 2^α . Now, applying $(\lambda,\tau) \in \mathrm{Aut}\, D_{2\alpha}$ to $<\rho>$, and remembering that λ is an odd number, we have :

$$<(\lambda,\tau):\rho> = <\rho^\lambda> = <\rho> \quad .$$

Then, $<\rho>$ is characteristic in $D_{2\alpha}$, i.e. it is mapped onto itself under all the automorphisms of $D_{2\alpha}$.

Application of (λ,τ) to $<\rho^2,\varepsilon>$ gives,

$$\begin{aligned} <(\lambda,\tau):\rho^2,\ (\lambda,\tau):\varepsilon> &= <\rho^{2^\lambda},\rho^\tau\varepsilon> \\ &= <\rho^2,\rho^\tau\varepsilon> \\ &= \begin{cases} <\rho^2,\varepsilon>, & \tau \text{ even} \\ <\rho^2,\rho\varepsilon>, & \tau \text{ odd.} \end{cases} \end{aligned} \tag{4.2}$$

On the other hand, the order of the intersections is :

$$\begin{aligned} |<\rho> \cap <\rho^2,\varepsilon>| = |<\rho> \cap <\rho^2,\rho\varepsilon>| &= |<\rho^2,\varepsilon> \cap <\rho^2,\rho\varepsilon>| \\ &= 2^{\alpha-1} \quad . \end{aligned}$$

Therefore, these three groups above considered are the unique subgroups of $D_{2\alpha}$ of order 2^{α} . This result can be used recursively for the dihedral subgroups $D_{2\alpha-1}$, $D_{2\alpha-2}$, ... Hence, it follows that the lattice of $D_{2\alpha}$ will be formed by blocks of the type shown in figure 2. From this figure, it is easy to obtain the complete lattice for $D_{2\alpha}$, which will consist in $2^{\alpha}-1$ interrupted sequences.

From equation (4.2) we see that the maximal subgroups of $D_{2\alpha}$, $<\varepsilon,\rho^2>$ and $<\rho\varepsilon,\rho^2>$, are related by the element $(1,1) \in \text{Aut } D_{2\alpha}$. On the other hand, there is always an element $(1,2^{r}) \in \text{Aut } D_{2\alpha}$ from which we get

$$<\varepsilon,\rho^{2^{r+1}}> \approx <\rho^{2^{r}}\varepsilon,\rho^{2^{r+1}}> \qquad \forall\ r\ , \text{ in the}$$

interval $0 \leq r \leq \alpha - 1$.

Then, the fundamental lattice of $D_{2\alpha}$ can be obtained from the blocks shown in figure 2, after deletion of the group $<\rho^{2^{k+1}},\ \rho^{2^{k}}\varepsilon>$.

Figure 3 shows the fundamental lattice for $D_{2\alpha}$ which is composed by α sequences of non isomorphic subgroups. Note that we take the axis of highest order in the same direction for all of the subgroups. Note also that we preserved ε as a generator of all of them. As we will see in the next section, these conventions will allow us to define in a general form the irreps adapted to the sequences $<\varepsilon,\rho^{2^{r}}> \supset <\rho^{2^{r}}>\ \forall\ r$.

Now we can write equation (4.1) in the following form :

$$<\varepsilon,\rho> = <\rho\varepsilon,\varepsilon,\rho^2> \quad . \tag{4.3}$$

As we see, the group $D_{2\alpha}$ can be given also by three generators such that, the different elements are expressed by $(\rho\varepsilon)^{\delta}\ \varepsilon^{\beta}\ (\rho^2)^{\gamma}$ with δ,β,γ integer positive numbers.

We shall now give an alternative definition of the group $D_{2\alpha}$ and its subgroups, using an arbitrary number of generators. If we write $\rho^{2^{s}}$ instead of ρ, equation (4.3) can be re-written as

$$<\varepsilon,\rho^{2^{s}}> = <\rho^{2^{s}}\varepsilon,\varepsilon,\rho^{2^{s+1}}> \quad . \tag{4.4}$$

Iterating this equation $r-s$ times, we have

$$<\varepsilon,\rho^{2^{s}}> = <\rho^{2^{s}}\varepsilon,\rho^{2^{s+1}}\varepsilon,\ldots,\varepsilon,\rho^{2^{r+1}}> \quad . \tag{4.5}$$

This equation allows us to introduce the notation

$$<\rho\varepsilon,\rho^2\varepsilon,\ldots,\varepsilon,\rho^{2^{r+1}}> \equiv$$

$$\equiv <\varepsilon,\rho> \supset <\varepsilon,\rho^2> \supset \ldots \supset <\varepsilon,\rho^{2^{r+1}}> \supset <\rho^{2^{r+1}}> , \tag{4.6}$$

which is also an alternative expression for the decomposition of a group into semidirect products of its subgroups, and is a compact form to express the sequences of the fundamental lattice of $D_{2\alpha}$, regarding that $<\varepsilon,\rho> \equiv \equiv <\varepsilon,\rho> \supset <\rho>$.

The importance of equation (4.6) rests on the fact that it also applies to crystallographic point groups - since they always can be decomposed into semidirect products containing some of their maximal subgroups[3] - as well as to nilpotent groups since their maximal subgroups, by definition, are always invariant.

(3) S.L.Altmann, Phil.Trans.Roy.Soc.A 255, 216-40 (1963).
S.L.Altmann, Rev.Mod.Phys. 35, 641-5 (1963).

There is also a practical advantage in this notation since every time we remove one generator on the left side of the bracket in equation (4.6), we get the set of generators identifying another maximal subgroup of the same sequence.

As we will see in section 5, this notation also introduces simplifications in the calculus of the irreps adapted to the sequences of a fundamental lattice.

5. IRREPS CALCULATION FOR THE GROUP $D_{2\alpha}$

We are going to apply the concepts developed in section 2 in order to obtain the irreps adapted in symmetry to the sequences of the group $D_{2\alpha}$.

If $D'_{2\alpha}$ is the commutator group of $D_{2\alpha}$ defined by

$$D'_{2\alpha} = \langle \{aba^{-1}b^{-1} | a,b \in D_{2\alpha}\} \rangle \quad ,$$

we have, $$D'_{2\alpha} = \langle \rho^2 \rangle \quad .$$

Then, the number of one-dimensional irreps of $D_{2\alpha}$ is $|D_{2\alpha}/D'_{2\alpha}| = 4$. On the other hand, remembering that $\rho\varepsilon = \varepsilon\rho^{-1}$, the classes of $D_{2\alpha}$ are $\mathbb{1}$; $\rho^{2^{\alpha-1}}$; (ρ^k,ρ^{-k}) for $0 < k < 2^{\alpha-1}$; $(\varepsilon,\rho^2\varepsilon,\ldots)$; $(\rho\varepsilon,\rho^3\varepsilon,\ldots)$. Therefore, using the theorem of Burnside[(4)] we conclude that the remainder irreps are bidimensional.

(4) A.A.Kirillow."Elements of the Theory of Representation".P.140. Springer-Verlag N.Y. (1976).

Now, returning to the fundamental lattice shown in figure 3, let us take the chain labelled by **a**, i.e. $\langle\varepsilon,\rho\rangle \supset \langle\rho\rangle \equiv \langle\varepsilon,\rho\rangle$. From $\rho^{2^\alpha} = \varepsilon^2 = 1$ and $\rho\varepsilon = \varepsilon\rho^{-1}$ we have, up to a fase factor,

$$ {}_{\mathbf{a}}E_k(\varepsilon) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad , \quad {}_{\mathbf{a}}E_k(\rho) = \begin{pmatrix} \omega & 0 \\ 0 & \omega^* \end{pmatrix}^k , \qquad (5.1) $$

where $\omega = \exp\{2^{1-\alpha}\pi i\}$.

We shall now calculate the isotropic group of the irreps:

$$ K_A(E_k) = \{ \varphi \in \mathrm{Aut}\ D_{2\alpha} \mid E_k^{\varphi} \sim E_k \} . $$

Using $\qquad E_k^{\varphi^{-1}}(g_i) = E_k(\varphi : g_i) \quad ,$

and from the results obtained in section 3, we have

$$ E_k^{(\lambda,\tau)^{-1}}(\rho) = E_k((\lambda,\tau):\rho) $$

$$ = E_{\lambda k}(\rho) \quad , \qquad (5.2) $$

where $\qquad \lambda k = \lambda k \ Mod\ 2^\alpha \quad , \text{ if } \ \lambda k \ Mod\ 2^\alpha \leq 2^{\alpha-1} \quad ,$

and $\qquad \lambda k = 2^\alpha - \lambda k \ Mod 2^\alpha \ , \text{if } \lambda k \ Mod\ 2^\alpha > 2^{\alpha-1} \quad .$

From equation (3.7) we get the elements to be used in (5.2). Therefore, it is immediate that the elements of $\langle(1,1)\rangle$ as well as those of $\langle(2^\alpha-1,0)\rangle$ belong to $K_A\ (E_k)$ for all k .

Now we write $k = 2^s\nu$, with ν an integer positive odd number and s ranging from zero to $\alpha - 2$.

From $k < 2^{\alpha-1}$, we have that $\nu < 2^{\alpha-1-s}$. Then, since $3^{2^{\alpha-2-s}} = 1 \; Mod \; 2^{\alpha-s}$ we finally conclude that the remaining elements of $K_A(E_k)$ are those belonging to $<(3^{2^{\alpha-2-s}},0)>$. These results allow us to express the isotropic group of the irreps as

$$K_A(E_{2^s\nu}) = <(1,1)> \circledS \{<(2^\alpha-1,0)> \otimes <(3^{2^{\alpha-2-s}},0)>\} \quad . \quad (5.3)$$

Since $<\rho>$ is characteristic in $D_{2\alpha}$, the isotropic group of the sequence $<\varepsilon,\rho>$ is

$$D_{2\alpha}S^{a} = \text{Aut } D_{2\alpha} \quad , \quad (5.4)$$

and from equation (2.3), we immediatly obtain

$$K_S^a(E_k) = K_A(E_k) \quad . \quad (5.5)$$

Equations (5.3) and (5.5) show that for the chain **a** we only need to calculate, for instance, the irreps E_{2^s} with $0 \leq s \leq \alpha - 2$ because the remaining ones can be obtained through the coset representatives of $K_S^a(E_k)$ in Aut $D_{2\alpha}$. This will be proved in appendix I, from the action of the automorphisms of $D_{2\alpha}$ which interchange classes. Particularly, relation $K_S^a(E_{2^{\alpha-2}}) = \text{Aut } D_{2\alpha}$ comes from the fact that $\rho^{2^{\alpha-1}}$ is the unique element, other than unit, that belongs to the center of $D_{2\alpha}$.

Now we wish to calculate the irreps adapted in symmetry to sequence $\mathbf{b} = <\rho\varepsilon,\varepsilon,\rho^2>$ using the results obtained for **a** .

First, we give the irreps adapted to

$<\varepsilon,\rho^2>$, which, in analogy to equation (5.1), are of the form

$$E_q(\varepsilon) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} , \quad E_q(\rho^2) = \begin{pmatrix} \omega & 0 \\ 0 & \omega^* \end{pmatrix}^{2q} , \quad (5.6)$$

where $0 < q < 2^{\alpha-2}$.

Second, taking into account that $\varepsilon\rho^{\ell}\varepsilon=\rho^{-\ell}$, we can write

$$U\, E_{2^{\alpha-1}-j}(\rho^2)\, U^{\dagger} = E_j(\rho^2) \quad , \quad (5.7)$$

$$U\, E_{2^{\alpha-1}-j}(\varepsilon)\, U^{\dagger} = E_j(\varepsilon) \quad , \quad (5.8)$$

where $0 < j < 2^{\alpha-2}$.

If now we apply these two transformations on the irreps given by equation (5.1), with $U = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ when $k > 2^{\alpha-2}$ and $U = (1/\sqrt{2})\begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}$ when $k = 2^{\alpha-2}$, we find the desired irreps which are shown in table 1 .

The isotropic group for the chain **b** is obtained in the same way. First we note that $<\rho^2>$ is characteristic in $D_{2\alpha}$ and $<\varepsilon,\rho^2>$ is a normal subgroup of $D_{2\alpha}$. Then, we only need to analyze the action of the elements $(3,0)$ and $(1,1)$ of Aut $D_{2\alpha}$ on ε and ρ^2. From equation (4.2),

$$<(3,0):\varepsilon\ ,\ (3,0):\rho^2> = <\varepsilon,\rho^2> \quad , \quad (5.9)$$

$$<(1,1):\varepsilon\ ,\ (1,1):\rho^2> = <\rho\varepsilon,\rho^2> \quad . \quad (5.10)$$

Hence, using equations (3.7) and (3.10),

$$D_{2^\alpha}S^b = \langle(1,2)\rangle \circledS \{\langle(2^\alpha-1,0)\rangle \otimes \langle(3,0)\rangle\} \quad . \quad (5.11)$$

Table 1 also includes the generators of the chain b_1 = $\langle\rho^2\varepsilon,\rho\varepsilon,\rho^2\rangle$, which is obtained from the application of the element $(1,1)$ on the generators of the sequence **b** .

The method applied to find the irreps adapted to chain **b** from those of chain **a** can be adopted to calculate the irreps adapted to chain **c** = $\langle\rho\varepsilon,\rho^2\varepsilon,\varepsilon,\rho^4\rangle$ and also can be used repeatedly until we obtain the irreps corresponding to the sequence $\langle\rho\varepsilon,\rho^2\varepsilon,\ldots,\varepsilon,\rho^{2^{\alpha-1}}\rangle$. However, it is important to bear in mind that in order to get the irreps adapted in symmetry to this last generic chain, the matrices corresponding to the elements ε and $\rho^{2^{\alpha-1}}$ must be diagonalized simultaneously. This can be done using the transformation matrix $U = (1/\sqrt{2})\begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}$.

We proceed now to apply the results to the group $D_8 \simeq D_{4d}$. The reader should notice that this group is convenient for application, since it is the group of lower order which has chains of types **b** and **c** . On the other hand, several compounds with this point symmetry are already known(5).

Figure 4 shows the lattice of interrupted sequences of the dihedral group D_8 and one fundamental lattice, together with the elements of the group Aut D_8

(5) D.L.Kepert. Prog.Inorg.Chem.24, 179 (1978).

which are needed to obtain the complete lattice from the fundamental one.

In order to obtain the irreps adapted to every sequence belonging to the lattice of D_8 we first write :

$$\mathrm{Aut}\ D_8 = \langle(1,1)\rangle \circledwedge \{\langle(7,0)\rangle \otimes \langle(3,0)\rangle\}$$

$$\mathrm{Inn}\ D_8 = \langle(1,2)\rangle \circledwedge \langle(7,0)\rangle$$

$$K_A(E_1) = \langle(1,1)\rangle \circledwedge \langle(7,0)\rangle$$

$$K_A(E_3) = K_A(E_1)$$

$$K_A(E_2) = \mathrm{Aut}\ D_8 \quad .$$

In particular, for each sequence of D_8 we have :

<u>$D_8 \supset C_8 = a$</u>

$$S^a = \mathrm{Aut}\ D_8 \quad .$$

Thus, there is only one chain of type a .

$$K_S(E_1) = \langle(1,1)\rangle \circledwedge \langle(7,0)\rangle \quad ,$$

$$K_S(E_3) = K_S(E_1) \ .$$

Since $(3,0) \in S^a$, we have $E_3 = E_1^{(3,0)}$.

$$K_S(E_2) = S^a \ .$$

Then, the irreps corresponding to chain a, are given by equation (5.1) with $\omega = \exp(i\pi/4)$.

$\underline{D_8 \supset D_4 \supset C_8 = b}$

$$S^b = \langle(1,2)\rangle \circledS \{\langle(7,0)\rangle \otimes \langle(3,0)\rangle\} \quad .$$

The element $(1,1)$ generates the isomorphic chain that we called b_1 .

$$K_S(E_1) = \text{Inn } D_8 \quad ,$$

$$K_S(E_3) = K_S(E_1) \quad .$$

Again, $E_3 = E_1^{(3,0)}$.

$$K_S(E_2) = S^b \quad .$$

The irreps adapted to b and b_1 are shown in table 1, where we must take $\omega = \exp(i\pi/4)$.

$\underline{D_8 \supset D_4 \supset D_2 = c}$

$$S^c = \langle(1,4)\rangle \otimes \langle(3,0)\rangle \otimes \langle(7,0)\rangle \quad .$$

The elements $(1,1)$, $(1,2)$ and $(1,3)$ generate three similar chains that we call c_1, c_2 and c_3 respectively.

$$K_S(E_1) = \langle(1,4)\rangle \otimes \langle(7,0)\rangle \quad ,$$

$$K_S(E_3) = K_S(E_1) \quad .$$

Again, $E_3 = E_1^{(3,0)}$.

$$K_S(E_2) = S^c \quad .$$

The irreps adapted in symmetry to chains c, c_1, c_2 and c_3 , are given in table 2 .

From the analysis of these three sequences we see that we can calculate, for all of them, E_3 from E_1 through the element $(3,0)$. This is a general property that applies to every sequence belonging to the groups D_{2^α} : knowing the irreps E_{2s}, we obtain the others just using the elements of the group $<(3,0)>$. This result follows from the fact that the groups D_{2^α} have subgroups given by $<\rho^{2^r}>$ and $<\varepsilon,\rho^{2^r}>$ with $0 \leq r \leq \alpha$ and, since 3 and 2^r are co-prime for all r, the element $(3,0)$ always belongs to the group of automorphisms of D_{2^r} .

6. DISCUSSION

The method developed in this work can be applied to any finite group G, following three *natural* steps.

1) DETERMINE Aut G

Since the elements of Inn G induce conjugations by $g \in G$ we need only to determine the representatives of the left cosets of Inn G in Aut G = $\oplus\, \varphi$ Inn G , which are of two types(6): those which do not interchange classes of G at all and, those which interchange, at least, two classes of G . Note that the interchanged classes must have the same number of elements of the same order.

(6) A.G.Kurosh, "The Theory of Groups".Ch.IV,Vol.I,Chelsea Publ.Co.N.Y.(1960).

In particular, Aut $D_{2\alpha}$ does not have elements of the first type : Let us call them φ_a . The classes of $D_{2\alpha}$ are $(\rho,\rho^{-1}),\ldots,(\varepsilon,\rho^2\varepsilon,\ldots),\ldots,(\rho\varepsilon,\rho^3\varepsilon,\ldots)$. In order to preserve these classes, the elements φ_a must be such that

$$\varphi_a : \rho \to \rho \text{ or } \rho^{-1}$$

$$\varphi_a : \rho^k\varepsilon \to \rho^{k+2\tau}\varepsilon \text{ or } \rho^{-k+2\tau}\varepsilon \quad .$$

From equation (3.9) we directly see that these mappings are induced by the automorphisms belonging to Inn $D_{2\alpha}$. Then , every outer automorphism of $D_{2\alpha}$ is of the second type. Under the action of the elements $(1,\tau)$,for odd τ , the class $(\varepsilon,\rho^2\varepsilon,\ldots)$ is mapped onto $(\rho\varepsilon,\rho^3\varepsilon,\ldots)$. In turn, the elements of $<(3,0)>$ map the classes $(\rho^{2^\delta\nu},\rho^{-2^\delta\nu})$ onto $(\rho^{2^\delta\nu'},\rho^{-2^\delta\nu'})$ for $(\nu\neq\nu')$.

The octahedral group is another interesting example. Since its classes are $\mathbb{1}$, $3C_2$, $6C_2'$, $6C_4$ and $8C_3$, it is impossible to induce an interchange of two of them by an outer automorphism.

Every element belonging to the group $\mathbf{O}$ can be obtained from the pair of generators C_4^x, C_4^z . Then, we must expect that we can also generate the group using the image pair $(C_4^x)^\varphi$, $(C_4^z)^\varphi \neq (C_4^x)^\varphi$. These elements must belong to the class $6C_4$; then, $|\text{Aut } \mathbf{O}| \leq 30$. Since the center of $\mathbf{O}$ is $Z(\mathbf{O}) = \{\mathbb{1}\}$, we have $|\text{Inn } \mathbf{O}| = |\mathbf{O}|/|Z(\mathbf{O})| = 24$.

Therefore, by the theorem of Lagrange[7], we have |Aut O| = 24k, (k integer). So, we conclude that the only possible value is k=1, i.e., Aut O = Inn O ≅ O . This result would have been obtained directly from the knowledge that O is isomorphic to S_4 and, therefore, it is a complete group[8].

From what we have seen, we are constrained to affirm that, although the investigation of the group of all automorphisms of a given group G is usually very difficult, the use of generators and a careful study of its corresponding transformations, introduce a great simplification in the algebraic calculation of Aut G . As a consequence, the determination of the automorphisms of crystallographic point groups becomes a nearly direct task.

2) OBTAIN THE FUNDAMENTAL LATTICE

It is important to note that there is not a general method to obtain the proper subgroups of a finite group.

Although the existence of subgroups can be investigated using the Lagrange theorem, it does not insure we are going to obtain the complete lattice.

Fortunately, all crystallographic point groups are Sylow's groups of order 3×2^m or 2^m ($m \geq 0$, integer). This fact allows us to use the powerful tool

(7) Reference (6), p.62.

(8) Reference (6), p.92.

that are Sylow's group theorems[9] in determining a group-subgroup structure.

On the other hand, from the knowledge of Aut G, and some arbitrary subgroup of G, we are able to obtain every subgroup and to identify the isomorphic ones.

3) DETERMINE THE IRREPS FOR THE SEQUENCES OF THE FUNDAMENTAL LATTICE

In section 2 we used a simple method to determine the irreps of the sequence $<\varepsilon,\rho>$ of the group $D_{2\alpha}$. In order to find the irreps adapted to any sequence $G \supset G_1 \supset \ldots \supset G_k$ of an arbitrary finite group G, it would be necessary to use the induction method. This method is simplified considerably when every member G_i of the sequence can be expressed as a product $G_i = G_{i+1} \otimes S_i$, where S_i is a cyclic group[10]. Fortunately, this condition is satisfied by at least one sequence of subgroups of all crystallographic point groups.

In appendix I, we show that the number of $\Gamma_n^{\varphi} \not\sim \Gamma_n$ induced by an outer automorphism $\varphi \in G$ is

(9) Cyril F. Gardiner. "A first course in group Theory", Ch.6. Springer-Verlag, N.Y.(1980).

(10) S.L.Altmann, "Induced Representations in Crystals and Molecules". P.268. Ac.Press (London)Ltd.(1977).

equal to the number of relations $(\varphi : C_k) \neq C_k$, where C_k are the classes of G . Then, it is not necessary to calculate all the irreps adapted to a given sequence, as was shown for $D_{2\alpha}$, where we only need to calculate the irreps E_{2s} for $0 \leq s \leq \alpha - 2$.

Once we have obtained the irreps adapted to a sequence of the fundamental lattice, we must determine the irreps adapted to the other sequences. We are compel to affirm that the method used in section 5 is more convenient than the induction method , because we are using it successfully in the calculation of the irreps adapted to the sequences of the group O_h .

We are now in a position to discuss the role played by the automorphisms of a group G in the Clebsch-Gordan coefficients of the group.

Let us consider a unitary matrix U, the elements of which are the Clebsch-Gordan coefficients of the group G . The reduction of the Kronecker product of the irreps of G may be written in the form :

$$U^{\dagger} \{ \Gamma_n(g) \otimes \Gamma_{n'}(g) \} U =$$

$$\bigoplus_{n''} \sigma(\Gamma_n \otimes \Gamma_{n'} | \Gamma_{n''}) \Gamma_{n''}(g) \quad ,$$

where σ is the frequency of $\Gamma_{n''}$ in the direct product of the representations.

According to $\Gamma_n(g) = \Gamma_n^{\varphi}(\varphi:g)$, we have

$$U^{\dagger}\ \Gamma_n^{\varphi}(g) \otimes \Gamma_{n'}^{\varphi}(g)\ U =$$

$$\bigoplus_{n''} \sigma(\Gamma_n \otimes \Gamma_{n'} |\ \Gamma_{n''})\Gamma_{n''}^{\varphi}(g) \qquad \forall\ \varphi \in \text{Aut } G.$$

It follows at once from this equation that

$$\sigma(\Gamma_n \otimes \Gamma_{n'} |\ \Gamma_{n''}) = \sigma(\Gamma_n^{\varphi} \otimes \Gamma_{n'}^{\varphi} |\ \Gamma_{n''}^{\varphi}) \quad .$$

When φ is an automorphism which interchanges classes, this relation between frequencies becomes an interesting non trivial equation. Moreover, we can write

$$<\Gamma_n\ \Gamma_{n'}\ \gamma_n\ \gamma_{n'} |\ b\ \Gamma_{n''}\gamma_{n''}> \quad =$$

$$<\Gamma_n^{\varphi}\ \Gamma_{n'}^{\varphi}\ \gamma_n^{\varphi}\ \gamma_{n'}^{\varphi} |\ b\ \Gamma_{n''}^{\varphi}\ \gamma_{n''}^{\varphi}>$$

where b runs from 1 to σ .

Clearly, this relation shows that a table of Clebsch-Gordan coefficients is greatly simplified when all the irreps of a group G are calculated from a minimal subset of irreps arbitrary prefixed.

For our particular case when $G = D_{2^\alpha}$, the minimal subset is that formed by the $\alpha-1$ irreps E_{2^s} , for $0 \leq s \leq \alpha-2$, from which we calculate the $2^{\alpha-1}$ irreps , just by application of the elements $(3^{\ell},0)$ and $(1,1)$ of Aut D_{2^α} .

Note also that the use of $\varphi \in$ Aut G for the group D_8 , directly evidences a symmetry by column exchange of the Clebsch-Gordan coefficients :

$$\langle E_1 \; E_2 \; \gamma \; \gamma \mid E_3 \; \gamma \rangle = \langle E_1^{(3,0)} E_2^{(3,0)} \gamma \; \gamma \mid E_3^{(3,0)} \gamma \rangle$$

$$= \langle E_3 \; E_2 \; \gamma \; \gamma \mid E_1 \; \gamma \rangle \quad ,$$

where γ denotes any component of the bases of the irreps E_k.

Clearly, we can extend the relations between the Clebsch-Gordan coefficients of a group **G** to any *nj* - symbol.

Finally, we turn our attention to the fact that the well known isomorphism $\mathbf{O} \simeq \mathbf{T_d}$ is generated by an element $\varphi \in \mathrm{Aut}\, \mathbf{O_h}$ such that $\varphi : C_2' \rightarrow IC_2'$, being C_2' an element belonging to the class $6C_2'$ of **O** . The group $\mathbf{T_d}$ can then be written as

$$\mathbf{T_d} = \mathbf{T} \circledS \langle IC_2' \rangle \simeq \mathbf{O} = \mathbf{T} \circledS \langle C_2' \rangle \quad ,$$

and, by direct application of the method developed in section 2, we obtain that the irreps adapted to the sequence $\mathbf{O_h} \supset \mathbf{T_d} \supset \mathbf{T} \supset \ldots$ can be taking also as those corresponding to the sequence $\mathbf{O_h} \supset \mathbf{O} \supset \mathbf{T} \supset \ldots$.

APPENDIX I

Theorem :

If we apply an outer automorphism $\varphi \in \mathrm{Aut}\, G$ on the irreps of a finite group G, the number of $(\varphi : \Gamma_n)$ inequivalent to Γ_n , is the same as the number of different relations induced by $\varphi : C_k \rightarrow C_{k'}$, $k \neq k'$.

Proof :

Let Γ_n be an irrep of G . Then,

$$\varphi : \Gamma_n(g_k) \rightarrow \Gamma_n(\varphi^{-1} : g_k) = \Gamma_n(g_{k'}) \ , \quad (g_k, g_{k'}) \in G \qquad (1)$$

Equation (1) shows that $\varphi : \Gamma_n$ is an irrep of G and then it is equivalent to some $\Gamma_{n'}$ of G, of the same dimension.

The characters of the irreps are such that,

$$\varphi : \chi_n(C_k) = \chi_{n'}(C_k) \ , \qquad (2)$$

$$= \chi_n(\varphi^{-1} : C_k) \ , \qquad (3)$$

$$= \chi_n(C_{k'}) \ . \qquad (4)$$

Equation (2) shows that φ induces permutations of the rows of the unitary matrix X the elements of which are $X_{nk} = (|C_k|/|G|)^{1/2} \chi_n(C_k)$. Equations (2) and (4) show that φ also induces permutations of the columns of the matrix X .

Now, if we define permutation matrices U and V, of elements $U_{ij} = \sum \delta_{in'} \delta_{jn}$ $V_{ij} = \sum \delta_{ik} \delta_{jk'}$, where the sums are over the pairs (n,n') and (k,k') obtained from $\varphi : \chi_n \to \chi_{n'}$ and $\varphi^{-1} : C_k \to C_{k'}$ respectively, relations (3) and (4) can be written as $U X = X V$. Since X is a unitary matrix, the matrices U and V have equal traces. Then, they exchange the same number of rows and columns of the matrix X. This proves the theorem.

Σ Sum

ACKNOWLEDGMENT

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CAPTION TO THE TABLES

TABLE 1 . Irreps symmetry adapted to the sequences $\mathbf{b}_1$ and $\mathbf{b}$, belonging to $D_{2\alpha}$ lattice. m runs from 1 to $2^{\alpha-2}-1$.

TABLE 2 . Irreps symmetry adapted to the sequences $\mathbf{c}$, $\mathbf{c}_1$, $\mathbf{c}_2$ and $\mathbf{c}_3$ corresponding to the group D_8 .

σ_i $(i=x,y,z)$ are the Pauli matrices.

σ_0 is the two-dimensional unit matrix.

TABLE 1

		GENERATORS		
CHAINS	b_1	$\rho^2\varepsilon$	$\rho\ \varepsilon$	ρ^2
	b	$\rho\ \varepsilon$	ε	ρ^2
REPRESENTATIONS	E_m	$\begin{pmatrix} 0 & \omega^m \\ \omega^{*m} & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$	$\begin{pmatrix} \omega & 0 \\ 0 & \omega^* \end{pmatrix}^{2m}$
	$E_{2^{\alpha-1}m}$	$\begin{pmatrix} 0 & \omega^{*m} \\ \omega^m & 0 \end{pmatrix}$		
	$E_{2^{\alpha-2}}$	$-i\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	$-\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$

TABLE 2

		GENERATORS			
CHAINS	c	$\rho\ \varepsilon$	$\rho^2\varepsilon$	ρ^4	ε
	c_1	$\rho^2\varepsilon$	$\rho^3\varepsilon$	ρ^4	$\rho\varepsilon$
	c_2	$\rho^3\varepsilon$	$\rho^4\varepsilon$	ρ^4	$\rho^2\varepsilon$
	c_3	$\rho^4\varepsilon$	$\rho^5\varepsilon$	ρ^4	$\rho^3\varepsilon$
REPRESENTATIONS	E_1	$(\sigma_z-\sigma_x)/\sqrt{2}$	$-\sigma_x$	$-\sigma_0$	σ_z
	E_3	$-(\sigma_z-\sigma_x)/\sqrt{2}$	$-\sigma_x$	$-\sigma_0$	σ_z
	E_2	σ_x	$-\sigma_z$	σ_0	σ_z

CAPTION TO THE FIGURES

FIGURE 1 . Relation $\Gamma(g_i) = \Gamma^{\varphi}(\varphi : g_i)$ valid for all $g \in G$ and $\varphi \in$ Aut G.

FIGURE 2 . Blocks to construct a lattice of a dihedral $D_{2\alpha}$.

FIGURE 3 . Fundamental lattice for a dihedral $D_{2\alpha}$.

FIGURE 4 . Lattice of the group D_8. Heavy lines show one of the possible fundamental lattices. The automorphisms needed to obtain the complete lattice from the fundamental one are indicated by arrows on the broken lines.

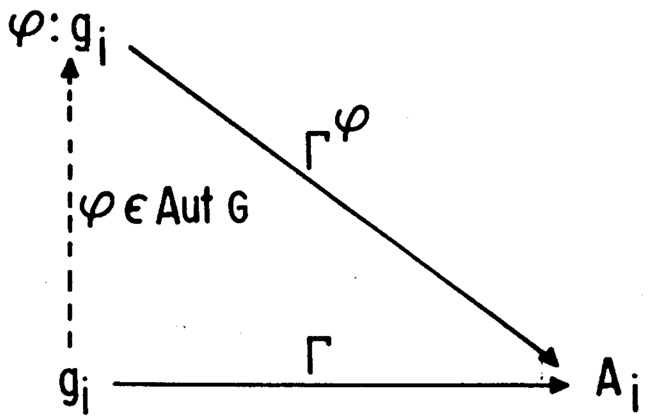


FIG.1

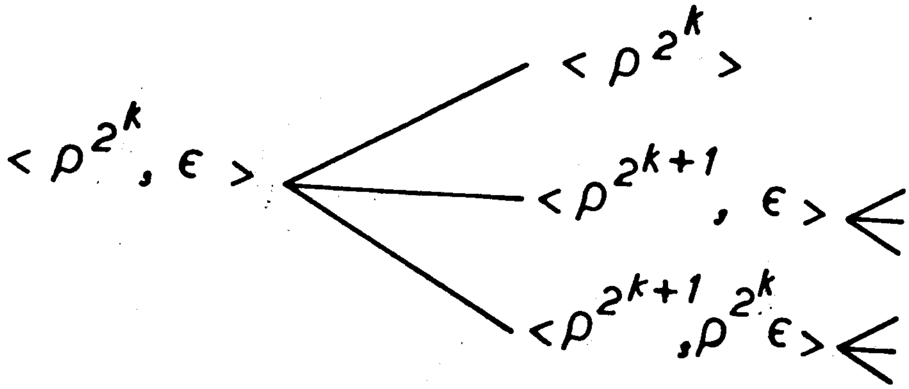


FIG.2

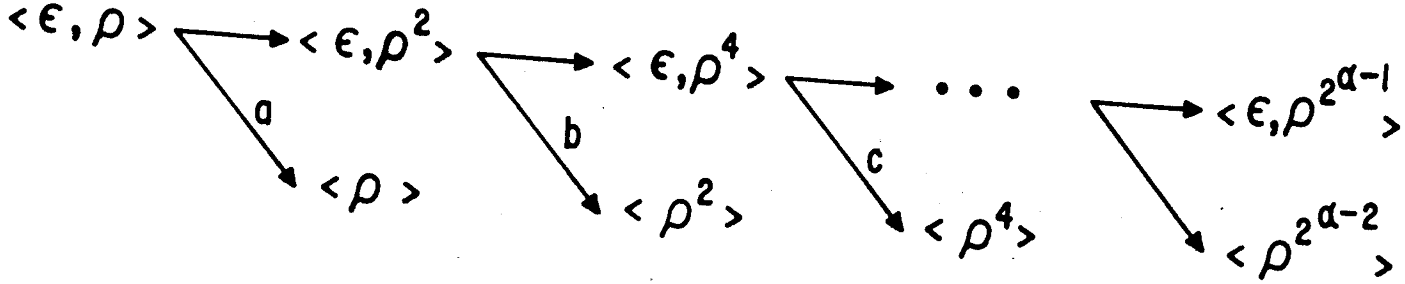
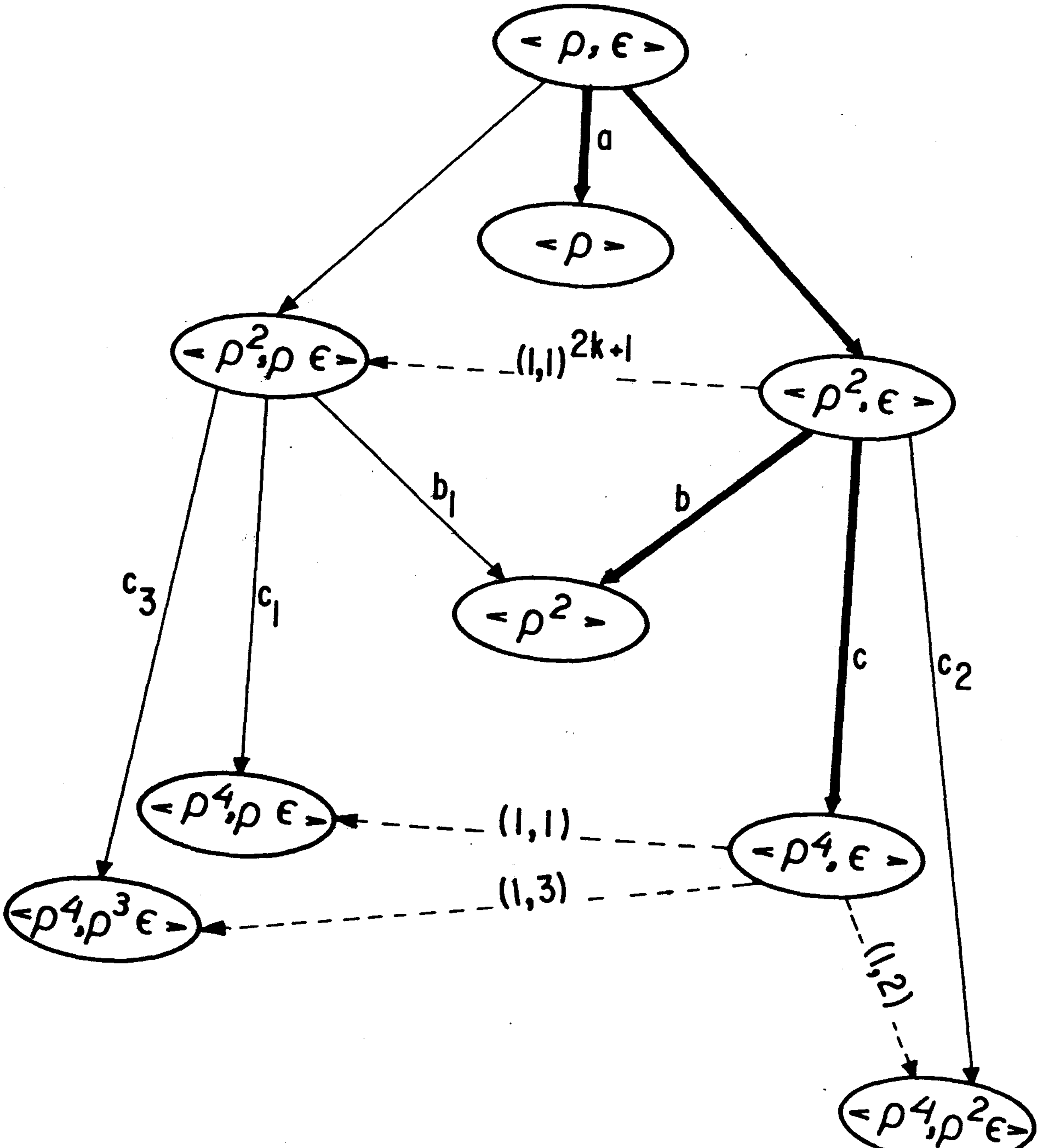


FIG. 3



< ρ, ε >
a
< ρ >
< ρ², ρ ε >
(1,1)^{2k+1}
< ρ², ε >
b₁
b
c₃
c₁
< ρ² >
c
c₂
< ρ⁴, ρ ε >
(1,1)
< ρ⁴, ε >
< ρ⁴, ρ³ ε >
(1,3)
(1,2)
< ρ⁴, ρ² ε >

FIG. 4