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THE SEQUENCES OF THE GROUP D_{4d}

by

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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 symmetries 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 was chosen, it leads to the elimination of the multiplicity problem, thereby solving the problem of labelling the basis states unambigously.

In this work, the chains of the non-crystallographic point group D_{4d} [1] are given in a form that simplifies symmetry adaptation and its application to molecular and solid state spectroscopy (calculation of symmetry adapted functions, representations, Clebsch-Gordan coefficients, etc.).

Using direct and semidirect products of subgroups of D_{4d} we can expand the chains in terms of the generators defined as follows.

Let $\langle\rho\rangle$ and $\langle\varepsilon\rangle$ be two groups which are generated by some arbitrary operations ρ and ε . Let n be any integer with $n \geq 2$. If $\rho^n = \varepsilon^2 = E$, $\varepsilon\rho = \rho^{-1}\varepsilon$ and $\langle\rho\rangle \cap \langle\varepsilon\rangle = E$,(where E is the identity element), it is well-known[2] that ρ and ε are the generators of a group $\langle\rho,\varepsilon\rangle$ with elements $\{E,\rho,\rho^2,\ldots,\rho^{n-1},\varepsilon,\rho\varepsilon,\rho^2\varepsilon,\ldots,\rho^{n-1}\varepsilon\}$.

It can be easily verified[3] that if n is even,

$$\begin{aligned}\langle \rho , \varepsilon \rangle &= \langle \rho \rangle \circledwedge \langle \varepsilon \rangle \\ &= (\langle \rho^2 \rangle \oplus \langle \rho^2 \rangle \rho) \circledwedge \langle \varepsilon \rangle \\ &= \langle \rho^2 , \varepsilon \rangle \circledwedge \langle \rho\varepsilon \rangle \quad . \end{aligned} \tag{1}$$

In the case when $n = 2^m$ ($m \geq 2$, integer), we obtain the recursion formulae

$$\langle \rho^{2^k} , \varepsilon \rangle = \langle \rho^{2^{(k+1)}} , \varepsilon \rangle \circledwedge \langle \rho^{2^k} \varepsilon \rangle \ , \quad k = 0,1,2,\ldots \tag{2}$$

In particular, let $C_\nu^{\vec{n}}$ be a rotation by $2\pi/\nu$ around the $\vec{n}$ axis. If we take $\rho = IC_8^{\vec{n}_1}$, $\varepsilon = IC_2^{\vec{n}_2}$ with $\vec{n}_1 . \vec{n}_2 = 0$ and $n_1^2 = n_2^2 = 1$, then $\langle \rho , \varepsilon \rangle = D_{4d}$.

Now, using equation (2) it is immediate that

$$\langle \rho , \varepsilon \rangle = \{ (\langle \rho^4 \rangle \otimes \langle \varepsilon \rangle) \circledwedge \langle \rho^2 \varepsilon \rangle \} \circledwedge \langle \rho\varepsilon \rangle \ , \tag{3}$$

where every group appearing in this equation is a cyclic group of order 2 .

Equation (3) can conveniently be rewritten as

$$\begin{aligned} D_{4d}(\rho,\varepsilon) &= \{ (C_2(\rho^4) \otimes C_s(\varepsilon)) \circledwedge C_s(\rho^2\varepsilon) \} \circledwedge C_2'(\rho\varepsilon) \\ &= D_{4d}(\rho^4,\varepsilon,\rho^2\varepsilon,\rho\varepsilon) \quad , \end{aligned} \tag{4}$$

and using, for example, table 19.6 of reference (3),

$$\begin{aligned} D_{4d}(\rho,\varepsilon) &= (C_{2v}(\rho^4,\varepsilon) \circledwedge C_s(\rho^2\varepsilon)) \circledwedge C_2'(\rho\varepsilon) \\ &= C_{4v}(\rho^4,\varepsilon,\rho^2\varepsilon) \circledwedge C_2'(\rho\varepsilon) \quad . \end{aligned} \tag{5}$$

Relations between multiple direct and semidirect products allow us to obtain alternative forms of equations (4) and (5) :

$$D_{4d}(\rho,\varepsilon) = \{(C_2(\rho^4) \otimes C_s(\rho^2\varepsilon)) \circledwedge C_s(\varepsilon)\} \circledwedge C_2'(\rho\varepsilon)$$
$$= (C_{2v}(\rho^4,\rho^2\varepsilon) \circledwedge C_s(\varepsilon)) \circledwedge C_2'(\rho\varepsilon)$$
$$= D_{4d}(\rho^4,\rho^2\varepsilon,\varepsilon,\rho\varepsilon) \quad , \qquad (6)$$

where we have used the fact that $\rho^4 \in Z(D_{4d})$, i.e. ρ^4 belongs to the centre of D_{4d} .

Equations (4), (5) and (6) give the right hand side chains of the lattice shown in figure 1. The map $\varphi : \rho^j \to \rho^j$, $\varphi : \rho^j\varepsilon \to \rho^{j+1}\varepsilon$ (j integer), acting on those chains, gives the left hand side members of the lattice. The central chain $D_{4d} \supset S_8$, corresponds to the first term in equation (1).

From figure 1 we observe that the structure of the sequences of D_{4d} is of the type $G_1 \supset G_2 \supset G_3 \supset G_4$, where $G_{i+1} \prec G_i$ since $(|G_i|/|G_{i+1}|) = 2$. This allows us to exhaust the subgroups and the chains of D_{4d} since we are able to use the theorem establishing that it is possible to generate an invariant subgroup of a finite group G, by using the class elements of G as a set of generators(4). Thus,

when $G = D_{4d}(\rho,\varepsilon)$
$= \langle\rho\rangle \circledwedge \langle\varepsilon\rangle$,

we have,

$$\langle\rho^4\rangle = Z(D_{4d}) \qquad (7.1)$$
$$\langle\rho,\rho^7\rangle = \langle\rho^3,\rho^5\rangle = S_8(\rho) \qquad (7.2)$$
$$\langle\rho^2,\rho^6\rangle = C_4(\rho^2) \qquad (7.3)$$
$$\langle\varepsilon,\rho^2\varepsilon,\rho^4\varepsilon,\rho^6\varepsilon\rangle = C_{4v}(\rho^2\varepsilon,\varepsilon,\rho^4) \qquad (7.4)$$
$$\langle\rho\varepsilon,\rho^3\varepsilon,\rho^5\varepsilon,\rho^7\varepsilon\rangle = D_4(\rho^3\varepsilon,\rho\varepsilon,\rho^4) \quad . \qquad (7.5)$$

If $G = C_{4v}(\rho^2\varepsilon,\varepsilon,\rho^4)$

$= <\rho^2> \otimes <\varepsilon>$,

we have

$$<\rho^4> = Z(C_{4v}) \quad (8.1)$$

$$<\rho^2,\rho^6> = C_4(\rho^2) \quad (8.2)$$

$$<\varepsilon,\rho^4\varepsilon> = C_{2v}(\varepsilon,\rho^4) \quad (8.3)$$

$$<\rho^2\varepsilon,\rho^6\varepsilon> = C_{2v}(\rho^2\varepsilon,\rho^4) \quad . \quad (8.4)$$

Finally,

if $G = D_4(\rho^3\varepsilon,\rho\varepsilon,\rho^4)$

$= <\rho^2> \otimes <\rho\varepsilon>$,

we have,

$$<\rho^4> = Z(D_4) \quad (9.1)$$

$$<\rho^2,\rho^6> = C_4(\rho^2) \quad (9.2)$$

$$<\rho\varepsilon,\rho^5\varepsilon> = D_2(\rho\varepsilon,\rho^4) \quad (9.3)$$

$$<\rho^3\varepsilon,\rho^7\varepsilon> = D_2(\rho^3\varepsilon,\rho^4) \quad . \quad (9.4)$$

The set of equations (7), (8) and (9) clearly exhausts all possible sequences of D_{4d}.

Some comments about these sequences are pertinent :

(i) The choice $\rho = IC_8^z$, $\varepsilon = IC_2^x$ is a convenient realization of D_{4d} because $\rho|\ell,m> = \lambda_1|\ell,m>$ and $\varepsilon|\ell,m> = \lambda_2|\ell,-m>$, where $\lambda_1 = \exp\{i(4\ell-m)/4\}$, $\lambda_2 = 1$. Then, the resulting irreducible representations(IR) are symmetry-adapted to the sequence $D_{4d} \supset S_8$.

(ii) It must be pointed out that in spite of the groups $<\varepsilon>$ and $<\rho^2\varepsilon>$ being related by the internal automorphism

$\rho\ \varepsilon\ \rho^{-1} = \rho^2\varepsilon$, they are presented as different final subgroups because they define different quantization axes[5] (C_2^x and C_2^{110} respectively).

(iii) It should be observed that the structure of figure 1 can obviously represent the sequences of subgroups of the group D_8 if $\rho = C_8^z$ and $\varepsilon = C_2^x$.

(iv) We have already remarked the importance of giving a chain in terms of appropriate generators. This is shown most conveniently by calculating, for instance, the IR adapted in symmetry to one of the sequences, say

$$D_{4d}(\rho\varepsilon,\rho^2\varepsilon,\rho^4,\varepsilon) \supset C_{4v}(\rho^2\varepsilon,\rho^4,\varepsilon) \supset C_{2v}(\rho^4,\varepsilon) \supset C_s(\varepsilon) \qquad (10)$$

from the IR adapted to the sequence $D_{4d} \supset S_8$. These IR are well-known[6] and they can be written in terms of Pauli matrices as

$$E_k(\rho) = \cos(k\pi/4)\ \sigma_0 + i\ \sin(k\pi/4)\ \sigma_z \qquad (11)$$
$$E_k(\varepsilon) = \sigma_x\ , \quad k = 1,2,3 \quad ,$$

where σ_0 is the unit 2x2 matrix and k labels the three two-dimensional IR of D_{4d} . Table 1 shows the matrix representation of the generators appearing in the sequence given by equation (10), calculated from equation (11), i.e., adapted in symmetry to $D_{4d} \supset S_8$.

In order to obtain from table 1 the IR adapted to the sequence given by (10), we must transform σ_x into σ_z . This can be done by a rotation in an angle π around the (101) axis, which transforms the vector $(\sigma_x,\sigma_y,\sigma_z)$ into

$(\sigma_z, -\sigma_y, \sigma_x)$ and separates E_2 into two one-dimensional representations corresponding to $C_{4v}(\rho^2\varepsilon, \rho^4, \varepsilon)$. The remaining two-dimensional representations E_1 and E_3 of D_{4d} correspond to E in C_{4v} since a rotation by π around the z axis acting on one of them transforms σ_y into $-\sigma_y$. Now, if we consider a clockwise rotation by $\pi/2$ around the z axis, it transforms every representation into a real matrix. Table 2 shows the resulting IR for D_{4d} after transformation.

This method could have been applied to every chain in figure 1 and it is so easy that saved the use of character tables.

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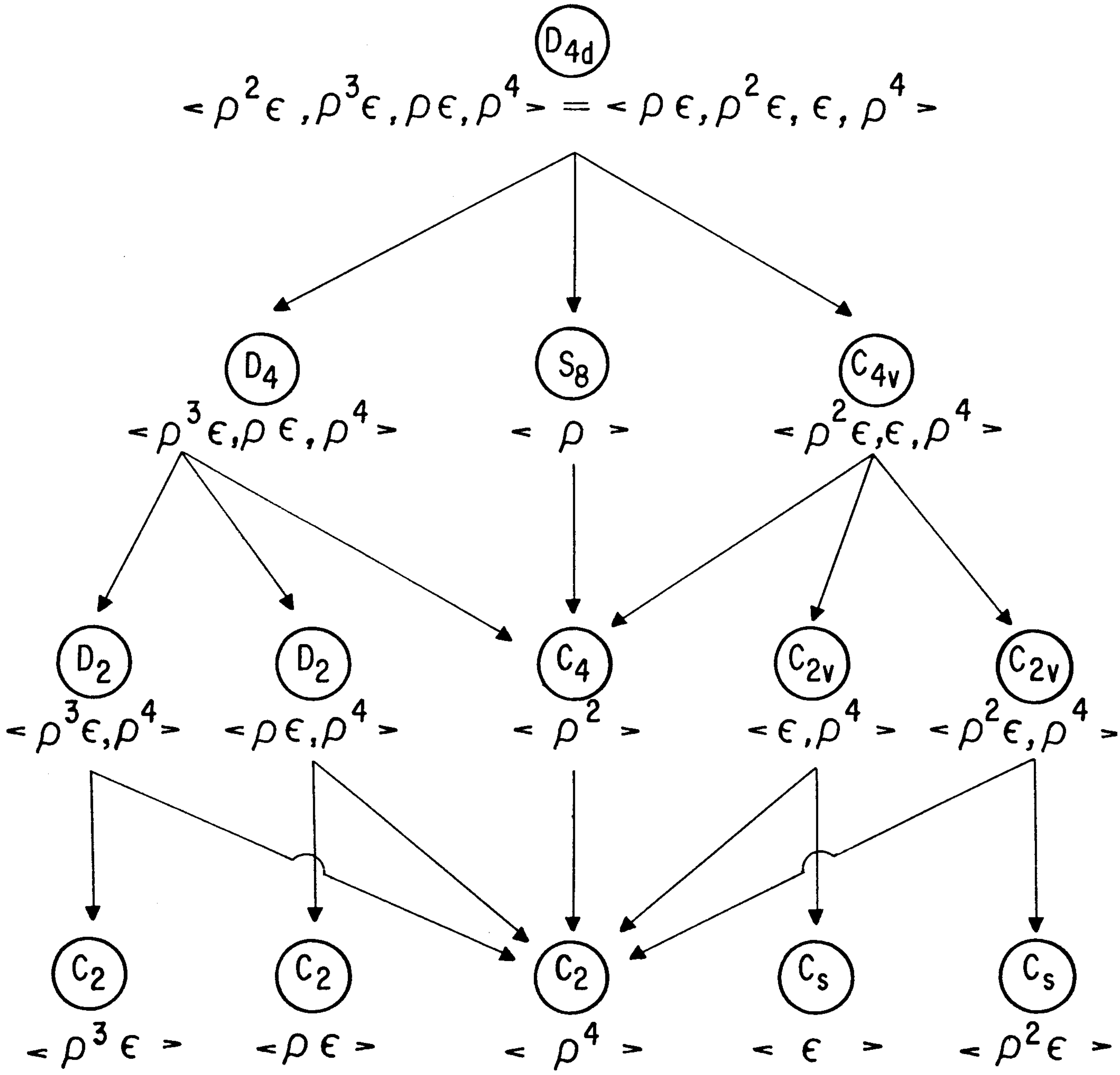

FIG. 1 – Lattice of the group D_{4d}

	$\rho\varepsilon$	$\rho^2\varepsilon$	ρ^4	ε
E_1	$(1/\sqrt{2})(\sigma_x - \sigma_y)$	$-\sigma_y$	$-\sigma_0$	σ_x
E_3	$-(1/\sqrt{2})(\sigma_x + \sigma_y)$	σ_y	$-\sigma_0$	σ_x
E_2	$-\sigma_y$	$-\sigma_x$	σ_0	σ_x

Table 1 . D_{4d} generators

	$\rho\varepsilon$	$\rho^2\varepsilon$	ρ^4	ε
E_1	$(1/\sqrt{2})(\sigma_z - \sigma_x)$	$-\sigma_x$	$-\sigma_0$	σ_z
E_3	$-(1/\sqrt{2})(\sigma_z - \sigma_x)$	$-\sigma_x$	$-\sigma_0$	σ_z
E_2	σ_x	$-\sigma_z$	σ_0	σ_z

Table 2 , D_{4d} generators after transformation

SYMBOLS AND NOTATION

$A \cap B$ Intersection (common elements) of A and B

$\in$ belongs to

$H \prec G$ H is an invariant subgroup of G

$Z(G)$ centre of G

$\oplus$ direct sum

$\owedge$ semidirect product

$\otimes$ direct product

$A \supset B$ B contained in A

$|G|$ order of G