dihedral

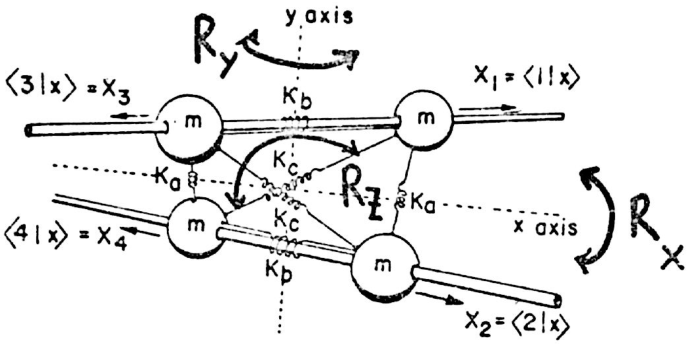
D_2 SYMMETRY EXAMPLE

$|1\rangle = |\mathbf{1}\rangle = \mathbf{1}|1\rangle$

$|2\rangle = |R_x\rangle = R_x|1\rangle$

$|3\rangle = |R_y\rangle = R_y|1\rangle$

$|4\rangle = |R_z\rangle = R_z|1\rangle$



Equation of Motion

$$-\begin{pmatrix} \langle 1|\ddot{x}\rangle \\ \langle 2|\ddot{x}\rangle \\ \langle 3|\ddot{x}\rangle \\ \langle 4|\ddot{x}\rangle \end{pmatrix} = \begin{pmatrix} A & a & b & c \\ a & A & c & b \\ b & c & A & a \\ c & b & a & A \end{pmatrix} \begin{pmatrix} \langle 1|x\rangle \\ \langle 2|x\rangle \\ \langle 3|x\rangle \\ \langle 4|x\rangle \end{pmatrix}$$

$A = a + b + c$

$a = k_a \dfrac{\cos^2(a,b)}{m}$

$b = k_b / m$

$c = k_c \dfrac{\cos^2(b,c)}{m}$

D_2:

$$\boxed{\begin{matrix} 1 & R_x & R_y & R_z \\ R_x & 1 & R_z & R_y \\ R_y & R_z & 1 & R_x \\ R_z & R_y & R_x & 1 \end{matrix}}$$

SPECTRAL DECOMPOSITION OF D_2

Minimal equation of R_x: $R_x^2 = 1$ | of R_y: $R_y^2 = 1$

R_x Idempotents:

$P^{x+} = (1 + R_x)/2$

$P^{x-} = (1 - R_x)/2$

$P^{x+} + P^{x-} = 1$

R_y Idempotents:

$P^{y+} = (1 + R_y)/2$

$P^{y-} = (1 - R_y)/2$

$P^{y+} + P^{y-} = 1$

two C_2 subalgebras

Splitting Into Irreducible Idempotents...

$$1 \cdot 1 = (P^{x+} + P^{x-})(P^{y+} + P^{y-}) = 1$$

$$1 = \underbrace{P^{x+}P^{y+} + P^{x+}P^{y-}}_{P^{x+}} + \underbrace{P^{x-}P^{y+} + P^{x-}P^{y-}}_{P^{x-}}$$

P^{y+} $\quad P^{y-}$

where:

$P^{x+}P^{y+} \equiv P^1 = (1 + R_x + R_y + R_z)/4$

$P^{x+}P^{y-} \equiv P^2 = (1 - R_x + R_y - R_z)/4$

$P^{x-}P^{y+} \equiv P^3 = (1 + R_x - R_y - R_z)/4$

$P^{x-}P^{y-} \equiv P^4 = (1 - R_x - R_y + R_z)/4$

$g =$	1	R_x	R_y	R_z	
$D^1(g) =$	1	1	1	1	A_1
$D^2(g) =$	1	-1	1	-1	B_2
$D^3(g) =$	1	1	-1	-1	B_3
$D^4(g) =$	1	-1	-1	1	B_1

$$P^k = \sum D^k(R_j)^* R_j / 4 \qquad R_j = \sum_k D^k(R_j) P^k$$

orthogonality
+ normalisation clear
(uniqueness not so simple)

Scanned by CamScanner

FIRST STEPS IN SPECTRAL DECOMPOSITION OF NON-ABELIAN GROUP → Find Commutative "class algebra"

	1	r	r^2	σ_1	σ_2	σ_3
1	1	r	r^2	σ_1	σ_2	σ_3
r	r	r^2	1	σ_3	σ_1	σ_2
r^2	r^2	1	r	σ_2	σ_3	σ_1
σ_1	σ_1	σ_2	σ_3	1	r	r^2
σ_2	σ_2	σ_3	σ_1	r^2	1	r
σ_3	σ_3	σ_1	σ_2	r	r^2	1

class-sum

	C_1	C_2	C_3
$1 = C_1$	1	C_2	C_3
$r + r^2 = C_2$	C_2	$21 + C_2$	$2C_3$
$\sigma_1 + \sigma_2 + \sigma_3 = C_3$	C_3	$2C_3$	$31 + 3C_2$

commutative

DEF: g' and g are in the same CLASS of $\mathcal{G} = \{1 \ldots g \ldots g' \ldots t \ldots\}$ if

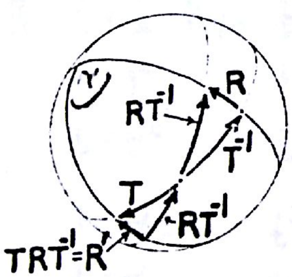
$$g' = t g t^{-1}$$

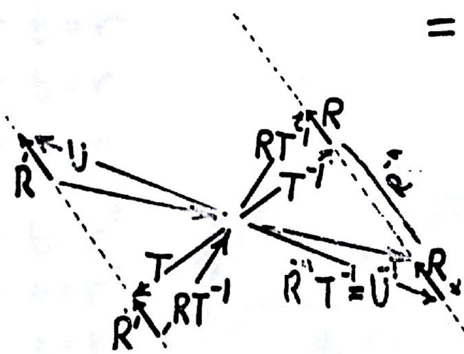
for ~~any~~ some t in $\mathcal{G}$.

C_{3v} Example:

$\sigma_2 = r \sigma_1 r^{-1}$

$\sigma_3 = r^{-1} \sigma_1 r$
$= \sigma_2 \sigma_1 \sigma_2^{-1}$





11-7

Obtaining Spectral Decomposition of a Class Algebra....

...finding minimal equations...

$$(C_3)^3 - 9C_3 = 0$$

finding roots..

$\ldots C_3^{(1)} = 3,\ C_3^{(2)} = -3,\ C_3^{(3)} = 0$

and projection ops...

$$\mathbb{P}^\alpha = \frac{\prod_{\gamma \neq \alpha} (C - C^{(\gamma)} 1)}{\prod_{\gamma \neq \alpha} (C^{(\alpha)} - C^{(\gamma)})}$$

	C_1	C_2	C_3
$1 = C_1$	1	C_2	C_3
C_2		$21 + C_2$	$2C_3$
C_3			$31 + 3C_2$

C_3: 3

$(C_3)^2 = 31 + 3C_2$ (not yet)

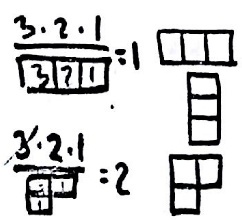
$(C_3)^3 = 3C_3 + 3C_2C_3 = 9C_3$ (OK!)

$\mathbb{P}^1 = (1 + C_2 + C_3)/6$

$\mathbb{P}^2 = (1 + C_2 - C_3)/6$

$\mathbb{P}^3 = (21 - C_2)/3$

11-10 hooklths → $\frac{n!}{}$



		1	C_2	C_3
A_1	(1)	1	1	1
A_2	(2)	1	1	-1
E	(3)	2	-1	0

(Construction of this CHARACTER Table will be explained later.)

Scanned by CamScanner

LECTURE 6
4/19/85

SOME BASIC GROUP THEORY: (SUBGROUPS AND CLASSES)

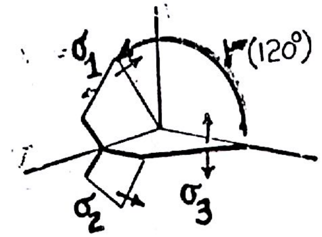
$$\boxed{\boxed{1}\ \boxed{r\quad r^2}}\quad \boxed{\sigma_1\ \sigma_2\ \sigma_3}$$

C_{3v} Group Classes

If $t=1$ then $t^{-1}\sigma_1 t=\sigma_1$
$t=\sigma_1$ $\quad t^{-1}\sigma_1 t=\sigma_1$

$t=\sigma_2$ $\quad t^{-1}\sigma_1 t=\sigma_3$
$t=r$ $\quad t^{-1}\sigma_1 t=\sigma_3$

$t=\sigma_3$ $\quad t^{-1}\sigma_1 t=\sigma_2$
$t=r^2$ $\quad t^{-1}\sigma_1 t=\sigma_2$



$r=\sigma_1\sigma_2$ $\quad r^{-1}=\sigma_2^{-1}\sigma_1^{-1}=\sigma_2\sigma_1$

$r^{-1}\sigma_1 r=\underbrace{(\sigma_2^{-1}\sigma_1^{-1})}_{r^{-1}}\sigma_1\underbrace{(\sigma_1\sigma_2)}_{r}$

$r^2=\sigma_1\sigma_3$

normalizer of σ_1

$$\boxed{\begin{matrix}1\\ \sigma_1\end{matrix}}\ \boxed{\begin{matrix}\sigma_2\\ r=\sigma_1\sigma_2\end{matrix}}\ \boxed{\begin{matrix}\sigma_3\\ r^2=\sigma_1\sigma_3\end{matrix}}$$

$\mathcal{H}\cdot C_2$ $\quad \mathcal{H}\sigma_2$ $\quad \mathcal{H}\sigma_3$

subgroup and right COSETS

$\sigma^2=1$, $\sigma^{-1}=\sigma$

If $t=1$ then $t^{-1}r\,t=r$
$t=r$ $\quad t^{-1}r\,t=r$
$t=r^2$ $\quad t^{-1}r\,t=r$

$t=\sigma_1$ $\quad t^{-1}r\,t=r^2$
$t=\sigma_3$ $\quad t^{-1}r\,t=r^2$
$t=\sigma_2$ $\quad t^{-1}r\,t=r^2$

$$\boxed{1\quad r\quad r^2}\ \mathcal{H}=C_3$$
$$\boxed{\sigma_1\quad \sigma_3=r\sigma_1\quad \sigma_2=r^2\sigma_1}\ \mathcal{H}\sigma_1$$

end Wed

Why class-sums commute with all the group elements.....

$$t\,c_g\,t^{-1}=t(g+g'+\ldots)t^{-1}=(g'+\ldots+g+\ldots)$$
$$=c_g$$

or: $\quad t\,c_g=c_g\,t \quad$ for all t in $\mathcal{G}$.

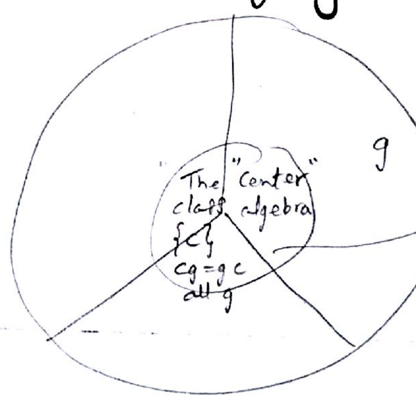
and: $\quad c_t c_g=c_g c_t$

Any all-commuting operator $\mathbf{C}=\sum_g \gamma_g\,\mathbf{g}$ ....

$t\mathbf{C}=\mathbf{C}t$ ... $\mathbf{C}=t\mathbf{C}t^{-1}$ ... for all t,

must be a combination of class-sums.

$$\mathbf{C}=\frac{1}{{}^\circ\mathcal{G}}\sum_t t\mathbf{C}t^{-1}=\frac{1}{{}^\circ\mathcal{G}}\sum_g\gamma_g\Big(\underbrace{\sum_t t\mathbf{g}t^{-1}}_{{}^\circ N\,\mathbf{c}_g}\Big)$$



C_{3v} gp. algebra

$C_1=1$
$C_2=r+r^2$
$C_3=\sigma_1+\sigma_2+\sigma_3$

11-8

11-9

Scanned by CamScanner

Derivation of Class Idempotents

$\mathbb{P}^j$

from three roots of $\mathbf{c}_3$

$c_3^{(1)}=3,\ c_3^{(2)}=-3,\ c_3^{(3)}=0$

1	c_2	c_3
c_2	$2\mathbf{1}+c_2$	$2c_3$
c_3	$2c_3$	$3\mathbf{1}+3c_2$

don't choose c_1 + c_2 – they're subalgebras!

$$\mathbb{P}^{(1)}=\frac{(\mathbf{c}_3-c^{(2)}\mathbf{1})(\mathbf{c}_3-c^{(3)}\mathbf{1})}{(c^{(1)}-c^{(2)})(c^{(1)}-c^{(3)})}=\frac{(\mathbf{c}_3+3\,\mathbf{1})(\mathbf{c}_3-0)}{(3+3)(3-0)}$$

$$=\frac{\mathbf{c}_3^2+3\mathbf{c}_3}{18}$$

$$\mathbb{P}^{(1)}=\frac{3\mathbf{1}+3\mathbf{c}_2+3\mathbf{c}_3}{18}=\frac{\mathbf{1}+\mathbf{c}_2+\mathbf{c}_3}{6}$$

$$\mathbb{P}^{(2)}=\frac{(\mathbf{c}_3-3\,\mathbf{1})(\mathbf{c}_3\quad)}{(-3-3)\ (-3)}=\frac{\mathbf{1}+\mathbf{c}_2-\mathbf{c}_3}{6}$$

$$\mathbb{P}^{(3)}=\frac{(\mathbf{c}_3-3\mathbf{1})(\mathbf{c}_3+3\mathbf{1})}{(0-3)(0+3)}=\frac{(\mathbf{c}_3^2-9\mathbf{1})}{-9}=\frac{2\mathbf{1}-\mathbf{c}_2}{3}$$

Spectral Decomposition of Classes

$$\mathbf{1}=\mathbf{c}_1=\mathbb{P}^{(1)}+\mathbb{P}^{(2)}+\mathbb{P}^{(3)}$$

$$r+r^2=\mathbf{c}_2=2\mathbb{P}^{(1)}-\mathbb{P}^{(2)}+2\mathbb{P}^{(3)}$$

$$\sigma_1+\sigma_2+\sigma_3=\mathbf{c}_3=3\mathbb{P}^{(1)}-3\mathbb{P}^{(2)}+0$$

$$\mathbb{P}^{(1)}=\tfrac{1}{6}\mathbf{1}+\tfrac{1}{6}\mathbf{c}_2+\tfrac{1}{6}\mathbf{c}_3$$

$$\mathbb{P}^{(2)}=\tfrac{1}{6}\mathbf{1}+\tfrac{1}{6}\mathbf{c}_2-\tfrac{1}{6}\mathbf{c}_3$$

$$\mathbb{P}^{(3)}=\tfrac{2}{3}\mathbf{1}-\tfrac{1}{3}\mathbf{c}_2$$

Scanned by CamScanner

SOME ALGEBRA THEORY FOR CLASS IDEMPOTENTS $\mathbb{P}^j$

i) With **n** class sums $\{c_1 = 1, c_2, \ldots, c_n\}$ its always possible to find **n** orthogonal $\{\mathbb{P}^{(1)}, \mathbb{P}^{(2)}, \ldots \mathbb{P}^{(n)}\}$

pf) The c_m's commute so the only possible foul-up would be a non-decomposable c_f i.e. a c_f with a repeated root in it's MinEq.

$$(c_f - \lambda 1)(\ldots)(c_f - \lambda' 1)^n(\ldots) = 0$$

$$\mathbf{n} \equiv (c_f - \lambda 1)(\ldots)(c_f - \lambda' 1)^{n-1}(\ldots) \neq 0$$

$$\mathbf{n} \cdot \mathbf{n} = 0 \quad \leftarrow \text{NILPOTENT}$$

if not zero

Not only is $\mathbf{n}$ nilpotent, but so is $\mathbf{n}G$ (I.N.Z.) where $G = \sum \gamma_g g$ is any combination of group ops.

$$\mathbf{n}G\,\mathbf{n}G = \mathbf{n}^2 GG = 0$$

and so is $N = \mathbf{n}\mathbf{n}^\dagger$ (I.N.Z.). But $\mathbf{n}\mathbf{n}^\dagger$ is Hermitian $N^\dagger = N$ and $(NN)_{ii} = 0 = \sum_j N_{ij} N_{ji}$

$$= \sum_j N_{ij} N_{ij}^* = \sum_j |N_{ij}|^2$$

implies $N_{ij} = 0 \ldots \therefore \boxed{\mathbf{n} = 0}$

Th) With n class sums $\{c_1 = 1, c_2, \ldots, c_n\}$ the n orthogonal idempotents $\{\mathbb{P}^{(1)}, \mathbb{P}^{(2)}, \ldots \mathbb{P}^{(n)}\}$ are unique.

proof) No $\mathbb{P}^{(j)}$ can "split" into

$$\mathbb{P}^{(j)} = I_1^{(j)} + I_2^{(j)}$$

where $I_k^{(j)}$ are orthogonal idempotent (non zero) combinations of c_m's, since we have only (n) c_m's and (n) $\mathbb{P}^{(j)}$'s, already.

But suppose another set of n $\mathbb{P}^{(j)\prime}$'s $\{\mathbb{P}^{(1)\prime}, \mathbb{P}^{(2)\prime}, \ldots \mathbb{P}^{(n)\prime}\}$. Can express $\mathbb{P}^{(j)}$'s in terms of them...

$$\mathbf{1} = \mathbb{P}^{(1)} + \mathbb{P}^{(2)} + \ldots + \mathbb{P}^{(n)} = \mathbb{P}^{(1)\prime} + \mathbb{P}^{(2)\prime} + \ldots + \mathbb{P}^{(n)\prime}$$

$$\mathbb{P}^{(1)} = \mathbb{P}^{(1)} + 0 + \ldots + 0 = \underbrace{\mathbb{P}^{(1)}\mathbb{P}^{(1)\prime} + \mathbb{P}^{(1)}\mathbb{P}^{(2)\prime} + \ldots + \mathbb{P}^{(1)}\mathbb{P}^{(n)\prime}}_{\text{only one can survive}}$$

Scanned by CamScanner

PART 2. GROUP ALGEBRA (Irreducible operators) of NON-ABELIAN POINT SYMMETRIES

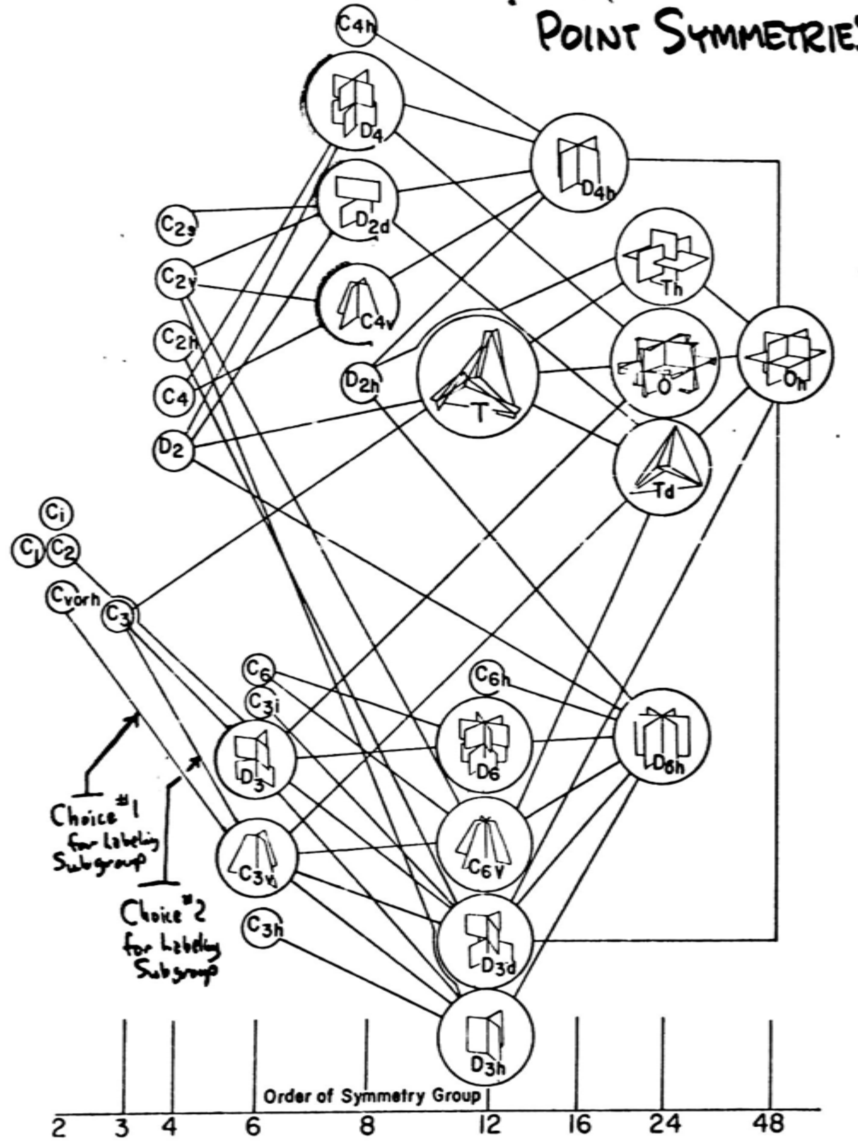


Fig 3.11 Crystal Point Symmetry Groups. Models are sketched in circles for the sixteen non-Abelian groups. 2-1

order of C_{3v} = 6 $\quad 1, \sigma_1, \sigma_2, \sigma_3, r, r^2$

" " center = 3 $\quad 1, \sigma_1+\sigma_2+\sigma_3, r, r^2$

" " rank = 4 $\quad 1, \sigma_1+\sigma_2+\sigma_3, r+r^2$

All-Commuting $\mathbb{P}^\alpha$ idempotents provide spectral decomposition of class-sums...

$$\mathbf{1} = \mathbf{C}_1 = \mathbb{P}^1 + \mathbb{P}^2 + \mathbb{P}^3$$

$$\mathbf{r}+\mathbf{r}^2 = \mathbf{C}_2 = 2\mathbb{P}^1 + 2\mathbb{P}^2 \cancel{+2}\mathbb{P}^3$$

$$\sigma_1+\sigma_2+\sigma_3 = \mathbf{C}_3 = 3\mathbb{P}^1 - 3\mathbb{P}^2$$

but <u>not all</u> group <u>operators</u> ...

... some $\mathbb{P}^\alpha$ must "split".

IRREDUCIBLE PROJECTION OPERATORS

1.) Find some group operator(s) which you would like to be "diagonal"

Say.... reflection σ_3 .... (Choice #1)

2.) Use their spectral decomposition...

example: $\mathbf{1} = P^1 + P^2 = (\mathbf{1}+\sigma_3)/2 + (\mathbf{1}-\sigma_3)/2$

to split the $\mathbb{P}$...

split!

$$\mathbf{1}\cdot\mathbf{1} = (P^1+P^2)(\mathbb{P}^1+\mathbb{P}^2+\mathbb{P}^3)$$
$$= P^1\mathbb{P}^1 + P^2\mathbb{P}^1 + P^1\mathbb{P}^2 + P^2\mathbb{P}^2 + P^1\mathbb{P}^3 + P^2\mathbb{P}^3$$
$$= \mathbb{P}^1 + 0 + 0 + \mathbb{P}^2 + \mathbf{P}^3_1 + \mathbf{P}^3_2$$

rank algebra

6 ? more 's do

not unique from here on

... 3

Scanned by CamScanner

$$1 = \mathbb{P}^1 + \mathbb{P}^2 + \underbrace{P_1^3 + P_2^3}_{\mathbb{P}^3} \qquad 2\mathbf{1} - \overbrace{r - r^2}^{c_2}$$

where:

symm split → $$P_1^3 = \overbrace{(1+\sigma_3)}^{P_1}\overbrace{(2\mathbf{1} - r - r^2)}^{\mathbb{P}^3}/6 = (2\mathbf{1} - r - r^2 - \sigma_1 - \sigma_2 + 2\sigma_3)/6$$

antisymm split → $$P_2^3 = \underbrace{(1-\sigma_3)}_{P_2}(2\mathbf{1} - r - r^2)/6 = (2\mathbf{1} - r - r^2 + \sigma_1 + \sigma_2 - 2\sigma_3)/6$$

3.) Use the resulting P_j^α to decompose the whole group...

$$g = \mathbf{1} g \mathbf{1} = (\mathbb{P}^1 + \mathbb{P}^2 + P_1^3 + P_2^3)\, g\, (\mathbb{P}^1 + \mathbb{P}^2 + P_1^3 + P_2^3)$$
$$= \mathbb{P}^1 g \mathbb{P}^1 + \mathbb{P}^2 g \mathbb{P}^2 + P_1^3 g P_1^3 + P_1^3 g P_2^3$$
$$+ P_2^3 g P_1^3 + P_2^3 g P_2^3$$

into ELEMENTARY PROJECTION OPERATORS (see App D)

$$P_{ij}^\alpha = P_i^\alpha g P_j^\alpha / \mathcal{D}_{ij}^\alpha(g) = P_{ji}^{\alpha\dagger}$$

normalized so that $$P_{ij}^\alpha P_{k\ell}^\beta = \delta^{\alpha\beta}\delta_{jk} P_{i\ell}.$$

12-4

$$\mathbb{P}^1\mathbb{P}^1 = \frac{(1+\sigma_3)}{2}\frac{(1 + \overbrace{r + r^2}^{c_2} + \overbrace{\sigma_1 + \sigma_2 + \sigma_3}^{c_3})}{6}$$
$$= (1 + r + r^2 + \sigma_1 + \sigma_2 + \sigma_3)/12$$
$$+ (\underbrace{\sigma_3}_{\sigma_3} + \underbrace{\sigma_3 r}_{\sigma_1} + \underbrace{\sigma_3 r^2}_{\sigma_2} + \underbrace{\sigma_3\sigma_1}_{r} + \underbrace{\sigma_3\sigma_2}_{r^2} + \underbrace{\sigma_3\sigma_3}_{1})/12$$

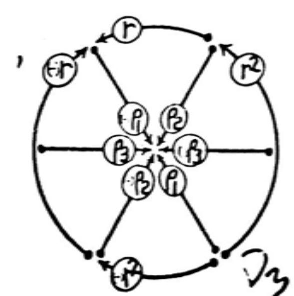
$$\therefore \mathbb{P}^1\mathbb{P}^1 = \mathbb{P}^1$$

$$\mathbb{P}^2\mathbb{P}^1 = (1 + r + r^2 + \sigma_1 + \sigma_2 + \sigma_3)/12$$
$$- (\sigma_3 + \sigma_1 + \sigma_2 + r + r^2 + 1)/12$$

$$\therefore \mathbb{P}^2\mathbb{P}^1 = 0$$

$$\mathbb{P}^2\mathbb{P}^2 = (1 + r + r^2 - \sigma_1 - \sigma_2 - \sigma_3)/12$$
$$- (\sigma_3 + \sigma_1 + \sigma_2 - r - r^2 - 1)/21$$

$$\therefore \mathbb{P}^2\mathbb{P}^2 = \mathbb{P}^2$$



12-2

$$\underbrace{(P_2^3 g P_1^3)(P_2^3 g P_1^3)}_{\text{orthog} = 0} = 0$$

irreducible projectors

Scanned by CamScanner

$$\mathbf{g} = \mathcal{D}^1(g)\,\mathbb{P}^1 + \mathcal{D}^2(g)\,\mathbb{P}^2 + \mathcal{D}^3_{11}(g)\,\mathbf{P}^3_{11} + \mathcal{D}^3_{12}(g)\,\mathbf{P}^3_{12}$$

$$\boxed{\mathbf{P}^3_1 \equiv \mathbf{P}^3_{11}}$$

$$P^3_{12} \sim P^3_1\, g\, P^3_2 \qquad + \mathcal{D}^3_{21}(g)\,\mathbf{P}^3_{21} + \mathcal{D}^3_{22}(g)\,\mathbf{P}^3_{22}$$

$$P_{12}P_{12} = 0$$

The coefficient matrix

$$\mathcal{D}^\alpha(g) = \begin{pmatrix} \mathcal{D}^\alpha_{11}(g) & \mathcal{D}^\alpha_{12}(g) & \cdots \\ \mathcal{D}^\alpha_{21}(g) & \mathcal{D}^\alpha_{22}(g) & \cdots \\ \vdots & \vdots & \end{pmatrix}$$

$$(P_{12})^2 = 0$$

NILPOTENT

is the (α)th IRREDUCIBLE REPRESENTATION (IR) of $\mathbf{g}$.

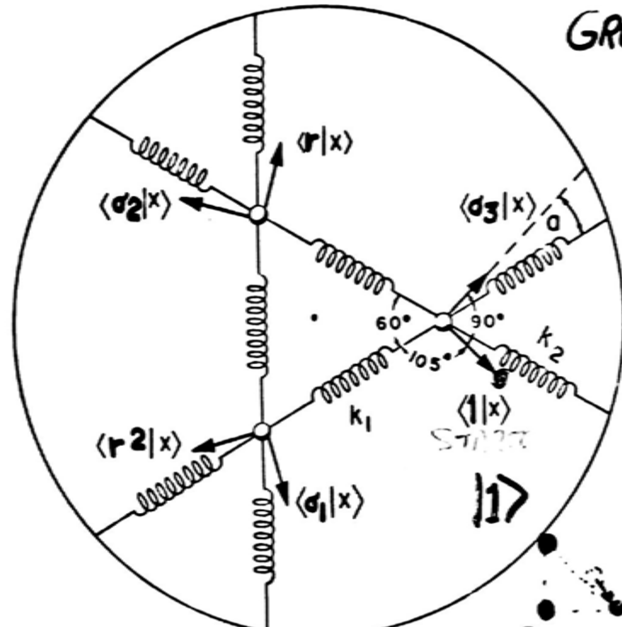
irrep.

If the dimension of $\mathcal{D}^\alpha$ is ℓ^α

then: $\text{ORDER OF GROUP } \mathcal{G} = {}^{o}\mathcal{G} = (\ell^\alpha)^2 + \ldots (\ell^\beta)^2 + \ldots$

$${}^{o}C_{3V} = 6 = 1^2 + 1^2 + 2^2$$

REGULAR REPRESENTATIONS: C_{3V} Example



GROUP BASIS:

$|r\rangle = r|1\rangle$

$|r^2\rangle = r^2|1\rangle$

$|\sigma_1\rangle = \sigma_1|1\rangle$

$\vdots$

$\langle r| = \langle 1|r^+$

$= \langle 1|r^{-1}$

$\vdots$

Scalar product: $\langle g|h\rangle = \delta_{g,h} = \delta_{g^{-1}h,1} = \langle 1|g^{-1}h|1\rangle$

Regular Rep.:

$$R_{hf}(g) = \langle h|g|f\rangle = \langle 1|h^{-1}gf|1\rangle$$

$$= \delta_{h^{-1}gf,1} = \delta_{g,hf^{-1}}$$

$$= f\left\{\boxed{\begin{matrix} 1 & r^2 & r & \sigma_1 & \sigma_2 & \sigma_3 \\ r & 1 & r^2 & \sigma_3 & \sigma_1 & \sigma_2 \\ r^2 & r & 1 & \sigma_2 & \sigma_3 & \sigma_1 \\ \sigma_1 & \sigma_3 & \sigma_2 & 1 & r & r^2 \\ \sigma_2 & \sigma_1 & \sigma_3 & r^2 & 1 & r \\ \sigma_3 & \sigma_2 & \sigma_1 & r & r^2 & 1 \end{matrix}}\right.$$

1·6..

example:

$$R(\sigma_3) = \begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix}$$

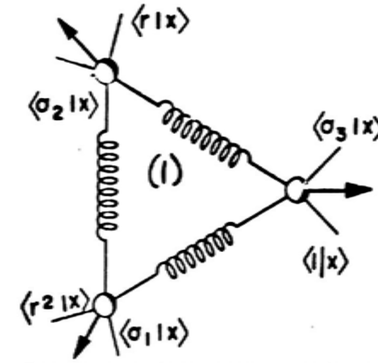
Scanned by CamScanner

order of the group

Note: $\text{Trace}\,\mathcal{R}(g) = \delta_{g,1}\,{}^{\circ}\!\mathcal{G} = \begin{cases} {}^{\circ}\mathcal{G} & g=1 \\ 0 & g\neq 1 \end{cases}$ (2-23)

σ_3 symm.

$\mathbb{P}^{(\alpha)}_{\bar{i}j}$ — global symm. (LAB); local symm. (Body)



$$\begin{pmatrix}1\\1\\1\\1\\1\\1\end{pmatrix}\begin{matrix}1\\r\\r^2\\\sigma_1\\\sigma_2\\\sigma_3\end{matrix}/\sqrt{6} = \begin{pmatrix}\langle 1|P^1\rangle\\\langle r|P^1\rangle\\\langle r^2|P^1\rangle\\\langle\sigma_1|P^1\rangle\\\langle\sigma_2|P^1\rangle\\\langle\sigma_3|P^1\rangle\end{pmatrix} \longleftrightarrow |\hat{P}^1\rangle$$

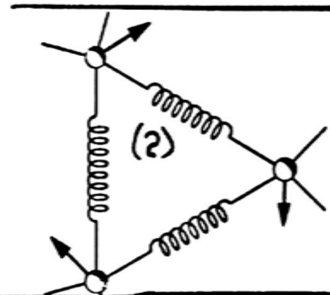
ELEMENTARY OPERATOR BASIS:

$$|\hat{P}^{\alpha}_{ij}\rangle \equiv \mathbf{P}^{\alpha}_{ij}|1\rangle/\sqrt{N^{\alpha}_{ij}} \qquad \left(\text{So: } \langle\hat{P}^{\alpha}_{ij}|\hat{P}^{\alpha}_{ij}\rangle = 1\right)$$

C_{3v} example:

$$\mathbb{P}^1 = (1+r+r^2+\sigma_1+\sigma_2+\sigma_3)/6 \qquad \langle\hat{P}^1| \to \frac{1\;1\;1\;1\;1\;1}{\sqrt{6}}$$

$$\mathbb{P}^2 = (1+r+r^2-\sigma_1-\sigma_2-\sigma_3)/6 \qquad \langle\hat{P}^2| \to \frac{1\;1\;1\;-1\;-1\;-1}{\sqrt{6}}$$



$$\begin{pmatrix}1\\1\\1\\-1\\-1\\-1\end{pmatrix}/\sqrt{6} \longrightarrow |\hat{P}^2\rangle$$

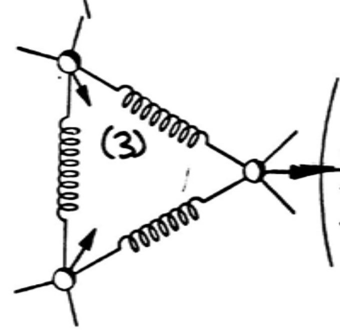
$$P^3_1 = P^3_1\,1\,P^3_1 \equiv P^3_{11} = (2\cdot1-r-r^2-\sigma_1-\sigma_2+2\sigma_3)/6 \qquad \langle\hat{P}^3_{11}| \to \frac{2\;-1\;-1\;-1\;-1\;2}{2\sqrt{3}}$$

$$P^3_2 = \;\equiv P^3_{22} = (2\cdot1-r-r^2+\sigma_1+\sigma_2-2\sigma_3)/6 \qquad \langle\hat{P}^3_{22}| \to \frac{2\;-1\;-1\;1\;1\;-2}{2\sqrt{3}}$$

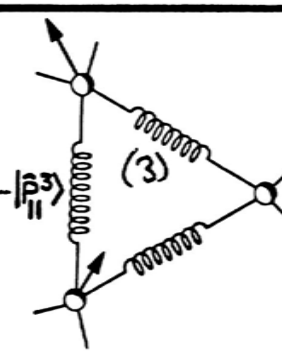
$$P^3_{12} \sim P^3_1\sigma_2P^3_2 = (-r+r^2-\sigma_1+\sigma_2)/4 \qquad \langle\hat{P}^3_{12}| \to \frac{0\;-1\;1\;-1\;1\;0}{2}$$

$$P^3_{21} \sim P^3_2\sigma_2P^3_1 = (r-r^2-\sigma_1+\sigma_2)/4 \qquad \langle\hat{P}^3_{21}| \to \frac{0\;1\;-1\;-1\;1\;0}{2}$$

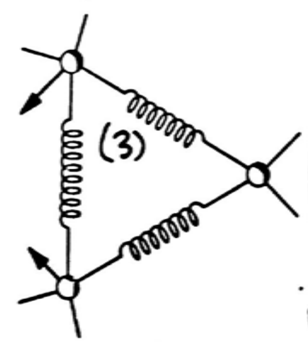
can use σ_1, σ_2, r or r^2



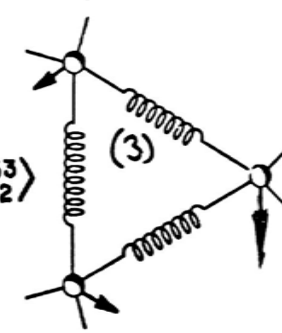
$$\begin{pmatrix}2\\-1\\-1\\-1\\-1\\2\end{pmatrix}/\sqrt{12} \to |\hat{P}^3_{11}\rangle$$



$$\begin{pmatrix}0\\1\\-1\\-1\\1\\0\end{pmatrix}/2 \to |\hat{P}^3_{21}\rangle$$



$$\begin{pmatrix}0\\-1\\1\\-1\\1\\0\end{pmatrix}/2 \to |\hat{P}^3_{12}\rangle$$



$$\begin{pmatrix}2\\-1\\-1\\1\\1\\-2\end{pmatrix}/\sqrt{12} \to |\hat{P}^3_{22}\rangle$$

Scanned by CamScanner

Orthogonality of $|\hat{P}^\alpha_{ij}\rangle = \mathbf{P}^\alpha_{ij}|1\rangle/\sqrt{N^\alpha_{ij}}$

$$\langle \hat{P}^\alpha_{ij}|\hat{P}^\beta_{k\ell}\rangle = \langle 1|\mathbf{P}^\alpha_{ji}\mathbf{P}^\alpha_{k\ell}|1\rangle\,\delta^{\alpha\beta}/\sqrt{N^\alpha_{ij}N^\alpha_{k\ell}}$$

$$= \langle 1|\,\mathbf{P}^\alpha_{j\ell}\,|1\rangle\,\delta_{ik}\,\delta^{\alpha\beta}/\sqrt{N^\alpha_{ij}N^\alpha_{i\ell}}$$

$$= \langle 1|\,P^\alpha_{jj}\,|1\rangle\,\delta_{j\ell}\,\delta_{ik}\,\delta^{\alpha\beta}/N^\alpha_{ij}$$

$$\boxed{N^\alpha_{ij} = N^\alpha = \langle 1|P^\alpha_{jj}|1\rangle} = \ell^\alpha/{}^\circ G$$

Understanding and Deriving IR $\mathcal{D}^\alpha_{ij}(g)$

$$g = \sum_{ij\alpha}\mathcal{D}^\alpha_{ij}(g)\,\mathbf{P}^\alpha_{ij}$$

So: $$g\,\mathbf{P}^\beta_{km} = \sum_{ij\alpha}\mathcal{D}^\alpha_{ij}(g)\,\mathbf{P}^\alpha_{ij}\,\mathbf{P}^\beta_{km}$$

$$g\,\mathbf{P}^\beta_{km} = \sum_i \mathcal{D}^\beta_{ik}(g)\,\mathbf{P}^\beta_{im}$$

$$\langle \hat{P}^\beta_{im}|g|\hat{P}^\beta_{km}\rangle = \mathcal{D}^\beta_{ik}(g)$$

12.9

$$\mathbf{r}|\hat{\mathbf{P}}^3_{11}\rangle = \mathbf{r}(2\mathbf{1} - \mathbf{r} - \mathbf{r}^2 - \sigma_1 - \sigma_2 + 2\sigma_3)|1\rangle/2\sqrt{3}$$

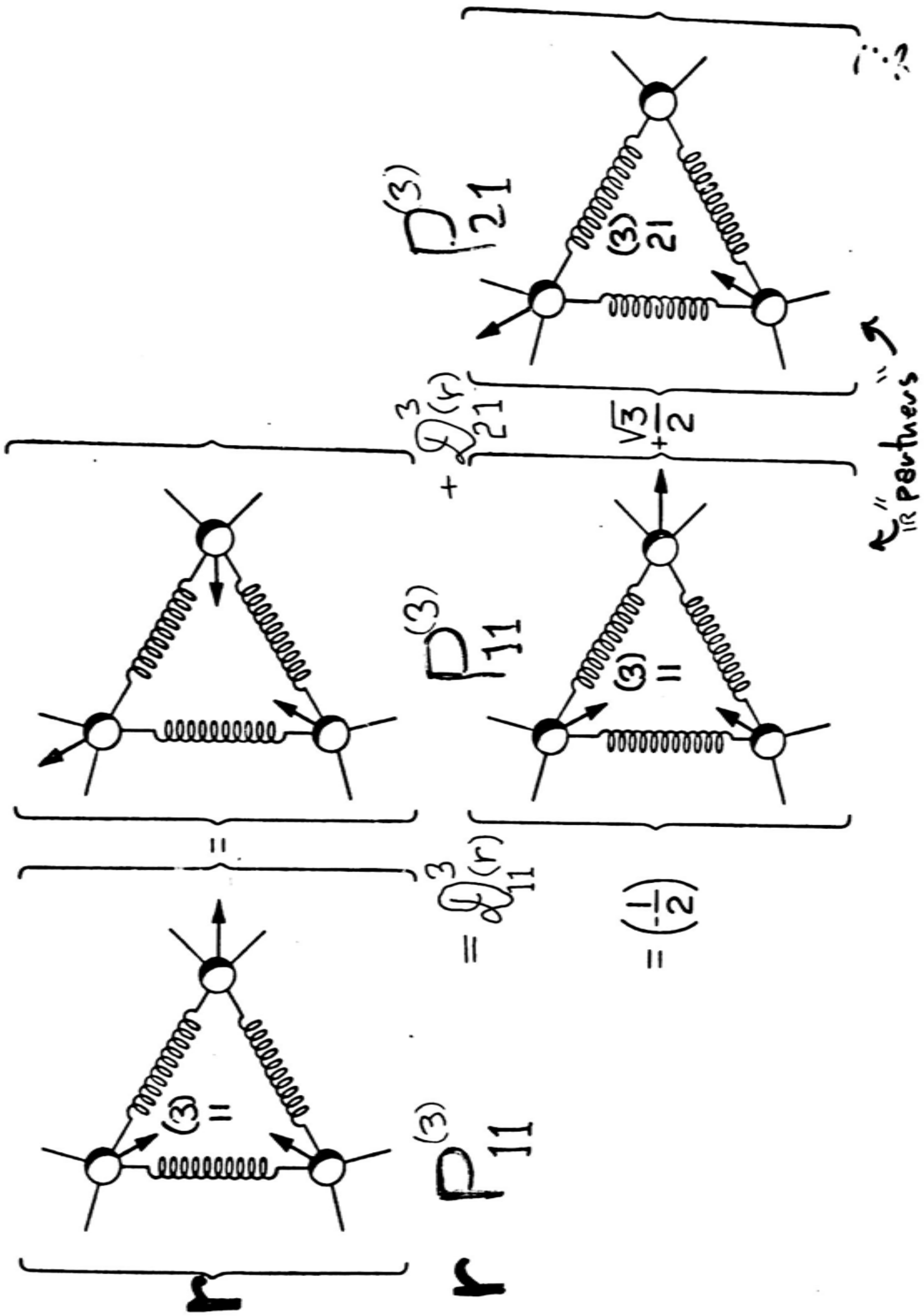
$$= (-\mathbf{1} + 2\mathbf{r} - \mathbf{r}^2 - \sigma_1 + 2\sigma_2 - \sigma_3)|1\rangle/2\sqrt{3} \rightarrow \begin{pmatrix}-1\\2\\-1\\-1\\2\\-1\end{pmatrix}/2\sqrt{3}$$

$$= \left(-\frac{1}{2}\right)\begin{pmatrix}2\\-1\\-1\\-1\\-1\\2\end{pmatrix}/2\sqrt{3} + \left(\frac{\sqrt{3}}{2}\right)\begin{pmatrix}0\\1\\-1\\-1\\1\\0\end{pmatrix}/2$$

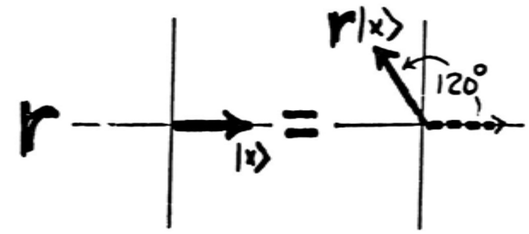
$$= \underbrace{\left(-\frac{1}{2}\right)}_{\mathcal{D}^3_{11}(\mathbf{r})}|\hat{\mathbf{P}}^3_{11}\rangle + \underbrace{\left(\frac{\sqrt{3}}{2}\right)}_{\mathcal{D}^3_{21}(\mathbf{r})}|\hat{\mathbf{P}}^3_{21}\rangle$$

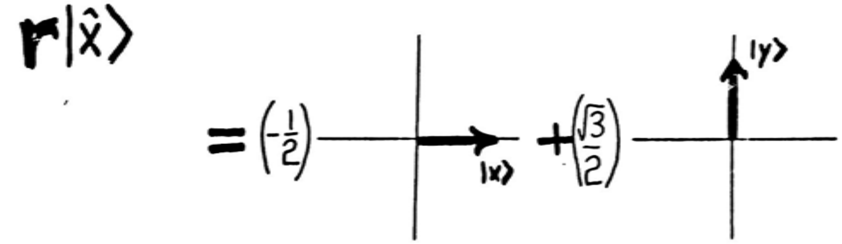
$$\mathcal{D}^3(\mathbf{r}) = \begin{pmatrix}-\frac{1}{2} & \\ \frac{\sqrt{3}}{2} & \end{pmatrix}$$

12.10 :



SIMPLE VECTOR INTERPRETATION (of E Irreducible Rep.

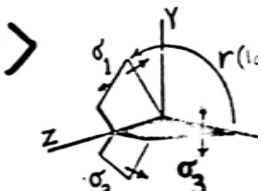




$$r|\hat{x}\rangle = \cos(120^\circ)|\hat{x}\rangle + \sin(120^\circ)|\hat{y}\rangle$$

$$r|\hat{y}\rangle = -\sin(120^\circ)|\hat{x}\rangle + \cos(120^\circ)|\hat{y}\rangle$$

$$\mathcal{D}^{E}(r) = \begin{pmatrix} \langle x|r|x\rangle & \langle x|r|y\rangle \\ \langle y|r|x\rangle & \langle y|r|y\rangle \end{pmatrix}$$



$\mathcal{D}^{E}(\sigma_2) =$ $\quad \mathcal{D}^{E}(\sigma_3)$

$$\mathcal{D}^{E}(1) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \mathcal{D}^{E}(r) = \begin{pmatrix} -1/2 & -\sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{pmatrix}, \mathcal{D}^{E}(r^2) = \begin{pmatrix} -1/2 & \sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \end{pmatrix}, \mathcal{D}^{E}(\sigma_1) = \begin{pmatrix} -1/2 & -\sqrt{3}/2 \\ -\sqrt{3}/2 & 1/2 \end{pmatrix}, \begin{pmatrix} -1/2 & \sqrt{3}/2 \\ \sqrt{3}/2 & 1/2 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\mathcal{D}^{A_2}(1) = (1) \quad \mathcal{D}^{A_2}(r) = (1) \quad \mathcal{D}^{A_2}(r^2) = (1) \quad \mathcal{D}^{A_2}(\sigma_1) = (-1) \quad \mathcal{D}^{A_2}(\sigma_2) = (-1), \mathcal{D}^{A_2}(\sigma_3)$$

$$\mathcal{D}^{A_1}(1) = (1) \quad (1) \quad (1) \quad (1) \quad (1) \quad (1)$$

	1	$r\ r^2$	$\sigma_1\sigma_2\sigma_3$	$= g$
A_1	1	1	1	$= \chi^{A_1}(g)$
A_2	1	1	-1	$= \chi^{A_2}(g)$
E	2	-1	0	$= \chi^{E}(g)$

Irrep. CHARACTERS

$$\chi^{\alpha}(g) = \text{TRACE}\ \mathcal{D}^{\alpha}(g)$$

PART 3. APPLICATION OF GROUP ALGEBRA

Decomposition of Non-Abelian Group $\mathcal{G}=\{1,g,\ldots\}$

The "all-commuting" $\mathbb{P}$: as many (α) as classes

$$1=\sum_{\alpha}\overbrace{\mathbb{P}^{\alpha}}$$

The "irreducible" P^{α}_j:

$$\left(P^{\alpha}_j=\mathbb{P}^{\alpha}P^{\alpha}_j=P^{\alpha}_j\mathbb{P}^{\alpha}\right)\qquad 1=\sum_{\alpha}P^{\alpha}_1+P^{\alpha}_2\ldots+P^{\alpha}_{\ell^{\alpha}}$$

Expanding g:

$$1\cdot g\cdot 1=g=\sum_{\alpha}\sum_{i}\sum_{j=1}\boxed{\begin{matrix}P^{\alpha}_i\, g\, P^{\alpha}_j\\ \mathcal{D}^{\alpha}_{ij}(g)\,P^{\alpha}_{ij}\end{matrix}}$$

in terms of "irreducible representations" and "elementary" operators:

$$\mathcal{D}^{\alpha}(g)=\begin{pmatrix}\mathcal{D}_{11}&\mathcal{D}_{12}&\cdots\\ \vdots&&\\ &\ell^{\alpha}\times\ell^{\alpha}&\end{pmatrix}\qquad \underset{\text{NILPOTENT}}{P_{12}P_{12}=0}\qquad \boxed{P^{\alpha}_{ij}P^{\alpha}_{km}=\delta_{jk}P^{\alpha}_{im}}$$

C_{3V} example:

	1	r	σ
(1)	1	1	1
(2)	1	1	-1
(3)	2	-1	0

$$1=\mathbb{P}^1+\mathbb{P}^2+\overbrace{\mathbb{P}^3}$$

$$\mathcal{D}^3(\sigma_3)=\begin{pmatrix}1&0\\0&-1\end{pmatrix}\qquad 1=\mathbb{P}^1+\mathbb{P}^2+P^3_1+P^3_2\qquad P_{11}P_{12}=P_{12}$$

$$\mathcal{D}^3(r)=\begin{pmatrix}-1/2&-\sqrt{3}/2\\ \sqrt{3}/2&-1/2\end{pmatrix}\qquad r=\mathcal{D}^1(r)\mathbb{P}^1+\mathcal{D}^2(r)\mathbb{P}^2+\mathcal{D}^3_{11}(r)P^3_{11}+\mathcal{D}_{12}P_{12}+\mathcal{D}_{21}P_{21}+\mathcal{D}_{22}P_{22}$$

Group-Operator Basis:

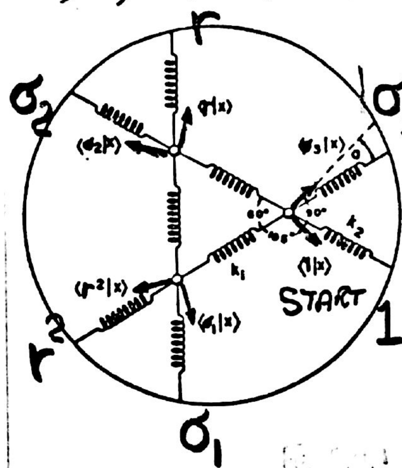
$$\ldots.\ |g\rangle=g\,|1\rangle$$

$$\underbrace{|1\rangle,|g\rangle,|g'\rangle\ldots}$$

dimension is order of group $=o\mathcal{G}=\ldots$

C_{3V} example: $\overbrace{6=oC_{3V}}$

$$|1\rangle,|r\rangle,|r^2\rangle,|\sigma_1\rangle,|\sigma_2\rangle,|\sigma_3\rangle.$$

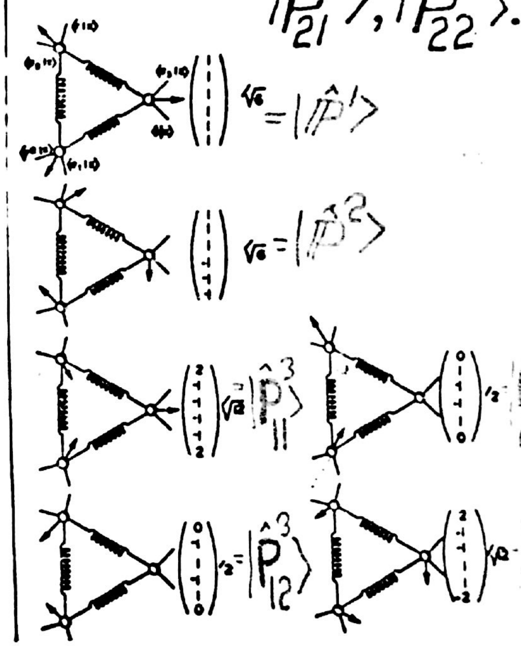


Projection Operator Basis:

$$\ldots.\ |\hat{P}^{\alpha}_{ij}\rangle=P^{\alpha}_{ij}|1\rangle/\sqrt{N}.$$

$$\underbrace{\ldots|\hat{P}^{\alpha}_{11}\rangle,|\hat{P}^{\alpha}_{12}\rangle\ldots|\hat{P}^{\alpha}_{1\ell^{\alpha}}\rangle,|\hat{P}^{\alpha}_{21}\rangle,\ldots}_{+(\ell^{\alpha})^2}\ \underbrace{|\hat{P}^{\beta}_{11}\rangle\ \vdots}_{+(\ell^{\beta})^2}$$

$$=\underbrace{1^2}_{|\hat{\mathbb{P}}^1\rangle}+\underbrace{1^2}_{|\hat{\mathbb{P}}^2\rangle}+\underbrace{2^2}_{|\hat{P}^3_{11}\rangle,|\hat{P}^3_{12}\rangle,|\hat{P}^3_{21}\rangle,|\hat{P}^3_{22}\rangle}.$$



Scanned by CamScanner

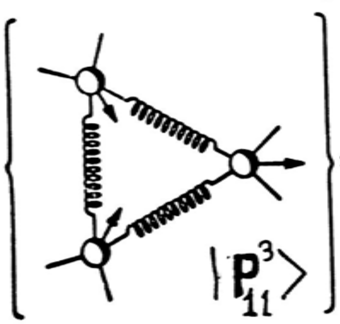
$$\mathbf{g} = \sum_\beta \sum_j \sum_k \mathcal{D}^\beta_{jk}(\mathbf{g})\, \mathbf{P}^\beta_{jk} \qquad (3.3.8)$$

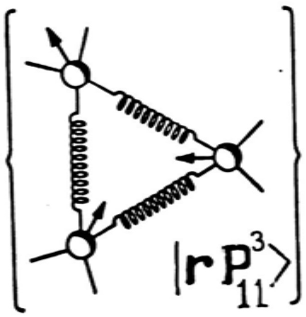
$$\mathbf{g}\mathbf{P}^\gamma_{\ell m} = \quad ,, \quad ,, \quad \mathbf{P}^\beta_{jk}\mathbf{P}^\gamma_{\ell m}$$

$$= \quad ,, \quad ,, \quad \delta^{\beta\gamma}\delta_{k\ell}\mathbf{P}^\gamma_{jm}$$

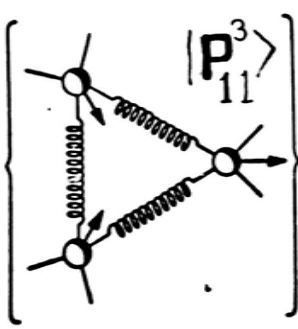
$$\mathbf{g}\mathbf{P}^\gamma_{\ell m} = \sum_j \mathcal{D}^\gamma_{j\ell}(\mathbf{g})\, \mathbf{P}^\gamma_{jm}$$

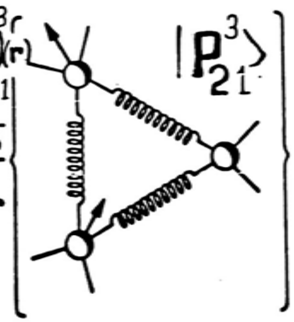
"Standard" Notation: $\mathbf{g}\psi^\gamma_\ell = \sum_j \mathcal{D}^\gamma_{j\ell}(\mathbf{g})\, \psi^\gamma_j$ or: $\langle \psi^\gamma_j, \mathbf{g}\psi^\gamma_\ell \rangle = \mathcal{D}^\gamma_{j\ell}(\mathbf{g})$

$\mathbf{r}$ 

$=$ 

(C_{3v} rotation example)

$= \underset{\mathcal{D}^3_{11}(\mathbf{r})}{\left(\frac{-1}{2}\right)}$ 

$+ \underset{\mathcal{D}^3_{21}(\mathbf{r})}{\frac{\sqrt{3}}{2}}$ 

Calculating P^β_{jk} given $\mathcal{D}^\beta$.....

... find coefficents $q_\mathbf{g}$ in $\mathbf{P}^\beta_{jk} = \sum_g q_\mathbf{g}\,\mathbf{g}$ ....

... $q_\mathbf{g} = \text{Trace}\,\mathcal{R}(\mathbf{g}^{-1}\mathbf{P}^\beta_{jk})/{}^\circ g$

where: $\mathbf{g}^{-1}\mathbf{P}^\beta_{jk} = \sum_i \mathcal{D}^\beta_{ij}(\mathbf{g}^{-1})\mathbf{P}^\beta_{ik} = \sum_i \mathcal{D}^{\beta *}_{ji}(\mathbf{g})\mathbf{P}^\beta_{ik}$ (by 3.

$q_\mathbf{g} = \sum_i \mathcal{D}^{\beta *}_{ji}(\mathbf{g})\ \text{Trace}\ \mathcal{R}(\mathbf{P}^\beta_{ik})/{}^\circ g$

$= \mathcal{D}^{\beta *}_{jk}(\mathbf{g})\ \ell^\beta/{}^\circ g$ (by inspecting

$$\boxed{\mathbf{P}^\beta_{jk} = (\ell^\beta/{}^\circ g)\sum_\mathbf{g} \mathcal{D}^{\beta *}_{jk}(\mathbf{g})\ \mathbf{g}}$$

$$\boxed{\mathbf{g} = \sum_{j\,\beta\,k} \mathcal{D}^\beta_{jk}(\mathbf{g})\ \mathbf{P}^\beta_{jk}}$$

Scanned by CamScanner

Representing Symmetry Operators

In Group Basis:

$$R^{g}_{fh}(g) = \langle f | g | h \rangle$$

$$|g\rangle^{\dagger} = \langle g| = \langle 1 | g^{\dagger}$$

$$R^{g}(\sigma_3) = \begin{array}{c} \begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix} \\ |1\rangle\, |r\rangle\, |r^2\rangle\, |\sigma_1\rangle\, |\sigma_2\rangle\, |\sigma_3\rangle \end{array}$$

$$\mathrm{Trace}\, R(g) = \begin{cases} {}^{\circ}g & g = 1 \\ 0 & g \neq 1 \end{cases}$$

for: $Q = q_1 1 + q_g g + \ldots$

$$q_1 = \mathrm{Trace}\, R(Q) / {}^{\circ}g$$

$$q_g = \mathrm{Trace}\, R(g^{-1} Q) / {}^{\circ}g$$

$\vdots$

$$\mathrm{Trace}\, R(P^{\alpha}_{jk}) = \begin{cases} \ell^{\alpha} & j = k \\ 0 & j \neq k \end{cases}$$

In Projection Basis:

$$R^{P}_{[P^{\alpha}_{ij}][P^{\beta}_{k\ell}]}(g) = \langle \hat{P}^{\alpha}_{ij} | g | \hat{P}^{\beta}_{k\ell} \rangle$$

$$R^{P}(g) = \begin{array}{c} \begin{pmatrix} \mathcal{D}^{1}(g) & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \mathcal{D}^{2}(g) & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \mathcal{D}^{3}_{11}(g) & \mathcal{D}_{12} & \cdot & \cdot \\ \cdot & \cdot & \mathcal{D}_{21} & \mathcal{D}_{22} & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \mathcal{D}^{3}_{11}(g) & \mathcal{D}_{12} \\ \cdot & \cdot & \cdot & \cdot & \mathcal{D}_{21} & \mathcal{D}_{22} \end{pmatrix} \\ |\hat{P}^1\rangle\, |\hat{P}^2\rangle\, |\hat{P}^3_{11}\rangle\, |\hat{P}_{21}\rangle\, |\hat{P}_{12}\rangle\, |\hat{P}_{22}\rangle \end{array}$$

$$R^{P}(P^{3}_{12}) = \begin{pmatrix} 0 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 0 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 0 & 1 & \cdot & \cdot \\ \cdot & \cdot & 0 & 0 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 0 & 1 \\ \cdot & \cdot & \cdot & \cdot & 0 & 0 \end{pmatrix}$$

(3.4.17)

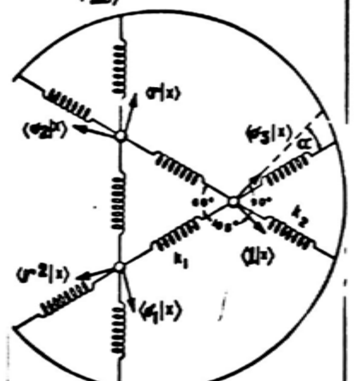
3.4

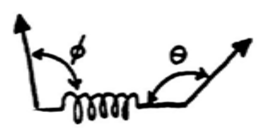
Representing System-Force Operator

In Group Basis:

$$\langle f | m\mathbf{a} | h \rangle =$$

$\lvert 1\rangle$	$\lvert r\rangle$	$\lvert r^2\rangle$	$\lvert \sigma_1\rangle$	$\lvert \sigma_2\rangle$	$\lvert \sigma_3\rangle$
$k_1 + k_2$	$\frac{k_1}{4}$	$\frac{k_1}{4}$	$k_1\frac{(2-\sqrt{3})}{4}$	$k_1\frac{(2+\sqrt{3})}{4}$	$k_1/2 + k_2 \sin 2\alpha$
$\frac{k_1}{4}$					





In Projection Basis:

$$\langle \hat{P}^{\alpha}_{ij} | m\mathbf{a} | \hat{P}^{\beta}_{k\ell} \rangle = \sum_{g} \langle 1 | \mathbf{a} | g \rangle \mathcal{D}^{\alpha *}_{j\ell}(g)\, \delta \ldots$$

$$\begin{array}{c} |\hat{P}^1\rangle\, |\hat{P}^2\rangle\, |\hat{P}^3_{11}\rangle\, |\hat{P}^3_{12}\rangle\, |\hat{P}^3_{21}\rangle\, |\hat{P}^3_{22}\rangle \\ \begin{pmatrix} 3k_1 + k_2(1+\sin 2\alpha) & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & k_2(1-\sin 2\alpha) & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 3k_1/4 + k_2(1+\sin 2\alpha) & 3k_1/4 & \cdot & \cdot \\ \cdot & \cdot & 3k_1/4 & 3k_1/4 + k_2(1-\sin 2\alpha) & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 3k_1/4 + k_2(1+\sin 2\alpha) & 3k_1/4 \\ \cdot & \cdot & \cdot & \cdot & 3k_1/4 & 3k_1/4 + k_2(1-\sin 2\alpha) \end{pmatrix} \end{array}$$

13.7

Scanned by CamScanner

Calculating P^{β}_{jk} given $\mathcal{D}^{\beta}$.....

... find coefficents q_{g} in $P^{\beta}_{jk} = \sum_{g} q_{g}\,\mathbf{g}$ ....

... $q_{g} = \text{Trace}\,\mathcal{R}(\mathbf{g}^{-1}P^{\beta}_{jk})/{}^{\circ}G$

where: $\mathbf{g}^{-1}P^{\beta}_{jk} = \sum_{i}\mathcal{D}^{\beta}_{ij}(\mathbf{g}^{-1})P^{\beta}_{ik} = \sum_{i}\mathcal{D}^{\beta*}_{ji}(\mathbf{g})P^{\beta}_{ik}$ (by 3.3.1)

$q_{g} = \sum_{i}\mathcal{D}^{\beta*}_{ji}(\mathbf{g})\ \text{Trace}\,\mathcal{R}(\mathbf{P}^{\beta}_{ik})/{}^{\circ}G$

$= \mathcal{D}^{\beta*}_{jk}(\mathbf{g})\ \ell^{\beta}/{}^{\circ}G$ (by inspecting 3.4.17 or (3.4.?))

$$\boxed{P^{\beta}_{jk} = (\ell^{\beta}/{}^{\circ}G)\sum_{\mathbf{g}}\mathcal{D}^{\beta*}_{jk}(\mathbf{g})\ \mathbf{g}}$$ (3.4.19)

$$\boxed{\mathbf{g} = \sum_{\beta}\sum_{j\,k}\mathcal{D}^{\beta}_{jk}(\mathbf{g})\ P^{\beta}_{jk}}$$ (3.3.?)

Normalization of $|\hat{P}^{\beta}_{jk}\rangle = P^{\beta}_{jk}|1\rangle/\sqrt{N^{\beta}}$ ...

N^{β} (or 0) $= \langle P^{\alpha}_{ij}|P^{\beta}_{k\ell}\rangle = \langle 1|P^{\alpha}_{ji}P^{\beta}_{k\ell}|1\rangle = \delta^{\alpha\beta}\delta_{ik}\langle 1|P^{\beta}_{j\ell}|1\rangle$

$= \delta^{\alpha\beta}\delta_{ik}\delta_{j\ell}\left[\langle 1|P^{\beta}_{jj}|1\rangle = \langle 1|\mathcal{D}^{\beta*}_{jj}(1)\mathbf{1} + \ldots|1\rangle\,\ell^{\beta}/{}^{\circ}G\right]$

$$\boxed{N^{\beta} = \ell^{\beta}/{}^{\circ}G}$$ (...

PROJECTION BASIS $|\hat{P}^{\alpha}_{ij}\rangle = P^{\alpha}_{ij}|1\rangle/\sqrt{N^{\alpha}}$ REPRESENTATIONS (GIVEN $\mathcal{D}^{\alpha}$)

Group Operators:

$\langle\hat{P}^{\alpha}_{ij}|\mathbf{g}|\hat{P}^{\beta}_{k\ell}\rangle = \langle 1|P^{\alpha}_{ji}\,\mathbf{g}\,P^{\beta}_{k\ell}|1\rangle/\sqrt{N^{\alpha}N^{\beta}}$

$= \sum_{i'}\mathcal{D}^{\beta}_{i'k}(\mathbf{g})\langle 1|P^{\alpha}_{ji}P^{\beta}_{i'\ell}|1\rangle/\sqrt{N^{\alpha}N^{\beta}}$ by

$= \delta^{\alpha\beta}\mathcal{D}^{\alpha}_{ik}\langle 1|P^{\alpha}_{j\ell}|1\rangle/N^{\alpha}$ by

$= \delta^{\alpha\beta}\mathcal{D}^{\alpha}_{ik}(\mathbf{g})\ \delta_{j\ell}$ by(...

System (Force-accel.) Operators:

$\langle\hat{P}^{\alpha}_{ij}|\mathbf{a}|\hat{P}^{\beta}_{k\ell}\rangle = \langle 1|\bar{P}^{\alpha\dagger}_{ij}\,\mathbf{a}\,P^{\beta}_{k\ell}|1\rangle/\sqrt{N^{\alpha}N^{\beta}}$

$= \langle 1|\mathbf{a}P^{\alpha}_{ji}P^{\beta}_{k\ell}|1\rangle/\sqrt{N^{\alpha}N^{\beta}}$ by COMMUTIVITY

$= \delta^{\alpha\beta}\langle 1|\mathbf{a}P^{\alpha}_{j\ell}|1\rangle\,\delta_{ik}/N^{\alpha}$ by

$= \delta^{\alpha\beta}\sum_{g}\mathcal{D}^{\alpha*}_{j\ell}(\mathbf{g})\langle 1|\mathbf{a}|\mathbf{g}\rangle\ \delta_{ik}$ by

Scanned by CamScanner

$$\mathbb{P}^{(1)} = \tfrac{1}{6}\mathbf{1} + \tfrac{1}{6}\mathbf{r} + \tfrac{1}{6}\mathbf{r}^2 + \tfrac{1}{6}\sigma_1 + \tfrac{1}{6}\sigma_2 + \tfrac{1}{6}\sigma_3 \qquad \mathbf{1} = \mathbb{P}^{(1)} + \mathbb{P}^{(2)} + P^{(3)}_{11} + P^{(3)}_{22}$$

$$\mathbb{P}^{(2)} = \tfrac{1}{6}\mathbf{1} + \tfrac{1}{6}\mathbf{r} + \tfrac{1}{6}\mathbf{r}^2 - \tfrac{1}{6}\sigma_1 - \tfrac{1}{6}\sigma_2 - \tfrac{1}{6}\sigma_3 \qquad \mathbf{r} = \mathbb{P}^{(1)} + \mathbb{P}^{(2)} - \tfrac{1}{2}P_{11} - \tfrac{\sqrt{3}}{2}P^{(3)}_{12} + \tfrac{\sqrt{3}}{2}P^{(3)}_{21} - \tfrac{1}{2}P_{22}$$

$$P^{(3)}_{11} = \tfrac{1}{3}\mathbf{1} - \tfrac{1}{6}\mathbf{r} - \tfrac{1}{6}\mathbf{r}^2 - \tfrac{1}{6}\sigma_1 - \tfrac{1}{6}\sigma_2 + \tfrac{1}{3}\sigma_3 \qquad \mathbf{r}^2 = \mathbb{P}^{(1)} + \mathbb{P}^{(2)} - \tfrac{1}{2}P_{11} + \tfrac{\sqrt{3}}{2}P_{12} - \tfrac{\sqrt{3}}{2}P_{21} - \tfrac{1}{2}P_{22}$$

$$P^{(3)}_{12} = -\tfrac{\sqrt{3}}{6}\mathbf{r} + \tfrac{\sqrt{3}}{6}\mathbf{r}^2 - \tfrac{\sqrt{3}}{6}\sigma_1 + \tfrac{\sqrt{3}}{6}\sigma_2 \qquad \sigma_1 = \mathbb{P}^{(1)} - \mathbb{P}^{(2)} - \tfrac{1}{2}P_{11} - \tfrac{\sqrt{3}}{2}P_{12} - \tfrac{\sqrt{3}}{2}P_{21} + \tfrac{1}{2}P_{22}$$

$$P^{(3)}_{21} = +\tfrac{\sqrt{3}}{6}\mathbf{r} - \tfrac{\sqrt{3}}{6}\mathbf{r}^2 - \tfrac{\sqrt{3}}{6}\sigma_1 + \tfrac{\sqrt{3}}{6}\sigma_2 \qquad \sigma_2 = \mathbb{P}^{(1)} - \mathbb{P}^{(2)} - \tfrac{1}{2}P_{11} + \tfrac{\sqrt{3}}{2}P_{12} + \tfrac{\sqrt{3}}{2}P_{21} + \tfrac{1}{2}P_{22}$$

$$P^{(3)}_{22} = \tfrac{1}{3}\mathbf{1} - \tfrac{1}{6}\mathbf{r} - \tfrac{1}{6}\mathbf{r}^2 + \tfrac{1}{6}\sigma_1 + \tfrac{1}{6}\sigma_2 - \tfrac{1}{3}\sigma_3 \qquad \sigma_3 = \mathbb{P}^{(1)} - \mathbb{P}^{(2)} + P_{11} - P_{22}$$

$$R(\mathbf{1}) = \begin{pmatrix} 1&\cdot&\cdot&\cdot&\cdot&\cdot\\ \cdot&1&\cdot&\cdot&\cdot&\cdot\\ \cdot&\cdot&1&\cdot&\cdot&\cdot\\ \cdot&\cdot&\cdot&1&\cdot&\cdot\\ \cdot&\cdot&\cdot&\cdot&1&\cdot\\ \cdot&\cdot&\cdot&\cdot&\cdot&1 \end{pmatrix}, \quad R(\mathbf{r}) = \begin{pmatrix} \cdot&\cdot&1&\cdot&\cdot&\cdot\\ 1&\cdot&\cdot&\cdot&\cdot&\cdot\\ \cdot&1&\cdot&\cdot&\cdot&\cdot\\ \cdot&\cdot&\cdot&\cdot&1&\cdot\\ \cdot&\cdot&\cdot&\cdot&\cdot&1\\ \cdot&\cdot&\cdot&1&\cdot&\cdot \end{pmatrix}, \quad R(\mathbf{r}^2) = \begin{pmatrix} \cdot&1&\cdot&\cdot&\cdot&\cdot\\ \cdot&\cdot&1&\cdot&\cdot&\cdot\\ 1&\cdot&\cdot&\cdot&\cdot&\cdot\\ \cdot&\cdot&\cdot&\cdot&\cdot&1\\ \cdot&\cdot&\cdot&1&\cdot&\cdot\\ \cdot&\cdot&\cdot&\cdot&1&\cdot \end{pmatrix},$$

$$R(\sigma_1) = \begin{pmatrix} \cdot&\cdot&\cdot&1&\cdot&\cdot\\ \cdot&\cdot&\cdot&\cdot&1&\cdot\\ \cdot&\cdot&\cdot&\cdot&\cdot&1\\ 1&\cdot&\cdot&\cdot&\cdot&\cdot\\ \cdot&1&\cdot&\cdot&\cdot&\cdot\\ \cdot&\cdot&1&\cdot&\cdot&\cdot \end{pmatrix}, \quad R(\sigma_2) = \begin{pmatrix} \cdot&\cdot&\cdot&\cdot&1&\cdot\\ \cdot&\cdot&\cdot&\cdot&\cdot&1\\ \cdot&\cdot&\cdot&1&\cdot&\cdot\\ \cdot&\cdot&1&\cdot&\cdot&\cdot\\ 1&\cdot&\cdot&\cdot&\cdot&\cdot\\ \cdot&1&\cdot&\cdot&\cdot&\cdot \end{pmatrix}, \quad R(\sigma_3) = \begin{pmatrix} \cdot&\cdot&\cdot&\cdot&\cdot&1\\ \cdot&\cdot&\cdot&1&\cdot&\cdot\\ \cdot&\cdot&\cdot&\cdot&1&\cdot\\ \cdot&1&\cdot&\cdot&\cdot&\cdot\\ \cdot&\cdot&1&\cdot&\cdot&\cdot\\ 1&\cdot&\cdot&\cdot&\cdot&\cdot \end{pmatrix}$$

$R(\mathbb{P}^{(1)}) =$ [illegible] $R(\mathbb{P}^{(2)})$ [illegible] $R(P^{(3)}_{11})$ [illegible] $R(P_{12})$ [illegible] $R(P_{21})$ [illegible] $R(P_{22})$ [illegible]

$$\underbrace{\begin{pmatrix} \frac{1}{\sqrt6}&\frac{1}{\sqrt6}&\frac{1}{\sqrt6}&\frac{1}{\sqrt6}&\frac{1}{\sqrt6}&\frac{1}{\sqrt6}\\ \frac{1}{\sqrt6}&\frac{1}{\sqrt6}&\frac{1}{\sqrt6}&-\frac{1}{\sqrt6}&-\frac{1}{\sqrt6}&-\frac{1}{\sqrt6}\\ \frac{1}{\sqrt3}&-\frac{1}{2\sqrt3}&-\frac{1}{2\sqrt3}&-\frac{1}{2\sqrt3}&-\frac{1}{2\sqrt3}&\frac{1}{\sqrt3}\\ 0&\frac12&\frac12&-\frac12&\frac12&0\\ 0&\frac12&-\frac12&-\frac12&\frac12&0\\ \frac{1}{\sqrt3}&-\frac{1}{2\sqrt3}&-\frac{1}{2\sqrt3}&\frac{1}{2\sqrt3}&\frac{1}{2\sqrt3}&-\frac{1}{\sqrt3} \end{pmatrix}}_{\mathcal{T}_R^\dagger} \underbrace{\begin{pmatrix} \text{regular representation} \\ R(g) \end{pmatrix}}_{R(g)} \underbrace{\begin{pmatrix} \frac{1}{\sqrt6}&\frac{1}{\sqrt6}&\frac{1}{\sqrt3}&0&0&\frac{1}{\sqrt3}\\ \frac{1}{\sqrt6}&\frac{1}{\sqrt6}&-\frac{1}{2\sqrt3}&\frac12&-\frac12&-\frac{1}{2\sqrt3}\\ \frac{1}{\sqrt6}&\frac{1}{\sqrt6}&-\frac{1}{2\sqrt3}&-\frac12&\frac12&-\frac{1}{2\sqrt3}\\ \frac{1}{\sqrt6}&-\frac{1}{\sqrt6}&-\frac{1}{2\sqrt3}&-\frac12&\frac12&\frac{1}{2\sqrt3}\\ \frac{1}{\sqrt6}&-\frac{1}{\sqrt6}&-\frac{1}{2\sqrt3}&\frac12&\frac12&\frac{1}{2\sqrt3}\\ \frac{1}{\sqrt6}&-\frac{1}{\sqrt6}&\frac{1}{\sqrt3}&0&0&-\frac{1}{\sqrt3} \end{pmatrix}}_{\mathcal{T}_R} = \begin{pmatrix} (\mathcal{D}^{(1)}(g)) & \cdot&\cdot&\cdot&\cdot&\cdot\\ \cdot&(\mathcal{D}^{(2)}(g))&\cdot&\cdot&\cdot&\cdot\\ \cdot&\cdot&\mathcal{D}^{(3)}_{11}(g)&\mathcal{D}_{12}&\cdot&\cdot\\ \cdot&\cdot&\mathcal{D}_{21}&\mathcal{D}_{22}&\cdot&\cdot\\ \cdot&\cdot&\cdot&\cdot&\mathcal{D}^{(3)}_{11}(g)&\mathcal{D}_{12}\\ \cdot&\cdot&\cdot&\cdot&\mathcal{D}_{21}&\mathcal{D}_{22} \end{pmatrix}$$

$$= A_1 \oplus A_2 \oplus 2E$$

$$\mathbb{P}^{(1)} = \tfrac{1}{6}\mathbf{1} + \tfrac{1}{6}\mathbf{r} + \tfrac{1}{6}\mathbf{r}^2 + \tfrac{1}{6}\sigma_1 + \tfrac{1}{6}\sigma_2 + \tfrac{1}{6}\sigma_3 \qquad \mathbf{1} = \mathbb{P}^{(1)} + \mathbb{P}^{(2)} + P^{(3)}_{11} + P^{(3)}_{22}$$

$$\mathbb{P}^{(2)} = \tfrac{1}{6}\mathbf{1} + \tfrac{1}{6}\mathbf{r} + \tfrac{1}{6}\mathbf{r}^2 - \tfrac{1}{6}\sigma_1 - \tfrac{1}{6}\sigma_2 - \tfrac{1}{6}\sigma_3 \qquad \mathbf{r} = \mathbb{P}^{(1)} + \mathbb{P}^{(2)} - \tfrac{1}{2}P_{11} - \tfrac{\sqrt{3}}{2}P^{(3)}_{12} + \tfrac{\sqrt{3}}{2}P^{(3)}_{21} - \tfrac{1}{2}P_{22}$$

$$P^{(3)}_{11} = \tfrac{1}{3}\mathbf{1} - \tfrac{1}{6}\mathbf{r} - \tfrac{1}{6}\mathbf{r}^2 - \tfrac{1}{6}\sigma_1 - \tfrac{1}{6}\sigma_2 + \tfrac{1}{3}\sigma_3 \qquad \mathbf{r}^2 = \mathbb{P}^{(1)} + \mathbb{P}^{(2)} - \tfrac{1}{2}P_{11} + \tfrac{\sqrt{3}}{2}P_{12} - \tfrac{\sqrt{3}}{2}P_{21} - \tfrac{1}{2}P_{22}$$

$$P^{(3)}_{12} = -\tfrac{\sqrt{3}}{6}\mathbf{r} + \tfrac{\sqrt{3}}{6}\mathbf{r}^2 - \tfrac{\sqrt{3}}{6}\sigma_1 + \tfrac{\sqrt{3}}{6}\sigma_2 \qquad \sigma_1 = \mathbb{P}^{(1)} - \mathbb{P}^{(2)} - \tfrac{1}{2}P_{11} - \tfrac{\sqrt{3}}{2}P_{12} - \tfrac{\sqrt{3}}{2}P_{21} + \tfrac{1}{2}P_{22}$$

$$P^{(3)}_{21} = +\tfrac{\sqrt{3}}{6}\mathbf{r} - \tfrac{\sqrt{3}}{6}\mathbf{r}^2 - \tfrac{\sqrt{3}}{6}\sigma_1 + \tfrac{\sqrt{3}}{6}\sigma_2 \qquad \sigma_2 = \mathbb{P}^{(1)} - \mathbb{P}^{(2)} - \tfrac{1}{2}P_{11} + \tfrac{\sqrt{3}}{2}P_{12} + \tfrac{\sqrt{3}}{2}P_{21} + \tfrac{1}{2}P_{22}$$

$$P^{(3)}_{22} = \tfrac{1}{3}\mathbf{1} - \tfrac{1}{6}\mathbf{r} - \tfrac{1}{6}\mathbf{r}^2 + \tfrac{1}{6}\sigma_1 + \tfrac{1}{6}\sigma_2 - \tfrac{1}{3}\sigma_3 \qquad \sigma_3 = \mathbb{P}^{(1)} - \mathbb{P}^{(2)} + P_{11} - P_{22}$$

$$R(\mathbf{1}) = \begin{pmatrix} 1&\cdot&\cdot&\cdot&\cdot&\cdot\\ \cdot&1&\cdot&\cdot&\cdot&\cdot\\ \cdot&\cdot&1&\cdot&\cdot&\cdot\\ \cdot&\cdot&\cdot&1&\cdot&\cdot\\ \cdot&\cdot&\cdot&\cdot&1&\cdot\\ \cdot&\cdot&\cdot&\cdot&\cdot&1 \end{pmatrix}, \quad R(\mathbf{r}) = \begin{pmatrix} \cdot&\cdot&1&\cdot&\cdot&\cdot\\ 1&\cdot&\cdot&\cdot&\cdot&\cdot\\ \cdot&1&\cdot&\cdot&\cdot&\cdot\\ \cdot&\cdot&\cdot&\cdot&1&\cdot\\ \cdot&\cdot&\cdot&\cdot&\cdot&1\\ \cdot&\cdot&\cdot&1&\cdot&\cdot \end{pmatrix}, \quad R(\mathbf{r}^2) = \begin{pmatrix} \cdot&1&\cdot&\cdot&\cdot&\cdot\\ \cdot&\cdot&1&\cdot&\cdot&\cdot\\ 1&\cdot&\cdot&\cdot&\cdot&\cdot\\ \cdot&\cdot&\cdot&\cdot&\cdot&1\\ \cdot&\cdot&\cdot&1&\cdot&\cdot\\ \cdot&\cdot&\cdot&\cdot&1&\cdot \end{pmatrix},$$

$$R(\sigma_1) = \begin{pmatrix} \cdot&\cdot&\cdot&1&\cdot&\cdot\\ \cdot&\cdot&\cdot&\cdot&1&\cdot\\ \cdot&\cdot&\cdot&\cdot&\cdot&1\\ 1&\cdot&\cdot&\cdot&\cdot&\cdot\\ \cdot&1&\cdot&\cdot&\cdot&\cdot\\ \cdot&\cdot&1&\cdot&\cdot&\cdot \end{pmatrix}, \quad R(\sigma_2) = \begin{pmatrix} \cdot&\cdot&\cdot&\cdot&1&\cdot\\ \cdot&\cdot&\cdot&\cdot&\cdot&1\\ \cdot&\cdot&\cdot&1&\cdot&\cdot\\ \cdot&\cdot&1&\cdot&\cdot&\cdot\\ 1&\cdot&\cdot&\cdot&\cdot&\cdot\\ \cdot&1&\cdot&\cdot&\cdot&\cdot \end{pmatrix}, \quad R(\sigma_3) = \begin{pmatrix} \cdot&\cdot&\cdot&\cdot&\cdot&1\\ \cdot&\cdot&\cdot&1&\cdot&\cdot\\ \cdot&\cdot&\cdot&\cdot&1&\cdot\\ \cdot&1&\cdot&\cdot&\cdot&\cdot\\ \cdot&\cdot&1&\cdot&\cdot&\cdot\\ 1&\cdot&\cdot&\cdot&\cdot&\cdot \end{pmatrix}$$

$R(\mathbb{P}^{(1)}) =$ [illegible] $R(\mathbb{P}^{(2)})$ [illegible] $R(P^{(3)}_{11})$ [illegible] $R(P_{12})$ [illegible] $R(P_{21})$ [illegible] $R(P_{22})$ [illegible]

$$\underbrace{\begin{pmatrix} \frac{1}{\sqrt6}&\frac{1}{\sqrt6}&\frac{1}{\sqrt6}&\frac{1}{\sqrt6}&\frac{1}{\sqrt6}&\frac{1}{\sqrt6}\\ \frac{1}{\sqrt6}&\frac{1}{\sqrt6}&\frac{1}{\sqrt6}&-\frac{1}{\sqrt6}&-\frac{1}{\sqrt6}&-\frac{1}{\sqrt6}\\ \frac{1}{\sqrt3}&-\frac{1}{2\sqrt3}&-\frac{1}{2\sqrt3}&-\frac{1}{2\sqrt3}&-\frac{1}{2\sqrt3}&\frac{1}{\sqrt3}\\ 0&-\frac12&\frac12&-\frac12&\frac12&0\\ 0&\frac12&-\frac12&-\frac12&\frac12&0\\ \frac{1}{\sqrt3}&-\frac{1}{2\sqrt3}&-\frac{1}{2\sqrt3}&\frac{1}{2\sqrt3}&\frac{1}{2\sqrt3}&-\frac{1}{\sqrt3} \end{pmatrix}}_{\mathcal{T}_a^\dagger} \underbrace{\begin{pmatrix} \text{acceleration} \\ \text{matrix} \\ \langle a \rangle \end{pmatrix}}_{\langle a \rangle} \underbrace{\begin{pmatrix} \frac{1}{\sqrt6}&\frac{1}{\sqrt6}&\frac{1}{\sqrt3}&0&0&\frac{1}{\sqrt3}\\ \frac{1}{\sqrt6}&\frac{1}{\sqrt6}&-\frac{1}{2\sqrt3}&\frac12&-\frac12&-\frac{1}{2\sqrt3}\\ \frac{1}{\sqrt6}&\frac{1}{\sqrt6}&-\frac{1}{2\sqrt3}&-\frac12&\frac12&-\frac{1}{2\sqrt3}\\ \frac{1}{\sqrt6}&-\frac{1}{\sqrt6}&-\frac{1}{2\sqrt3}&-\frac12&\frac12&\frac{1}{2\sqrt3}\\ \frac{1}{\sqrt6}&-\frac{1}{\sqrt6}&-\frac{1}{2\sqrt3}&\frac12&\frac12&\frac{1}{2\sqrt3}\\ \frac{1}{\sqrt6}&-\frac{1}{\sqrt6}&\frac{1}{\sqrt3}&0&0&-\frac{1}{\sqrt3} \end{pmatrix}}_{\mathcal{T}_a} = \begin{pmatrix} [illegible] & \cdot&\cdot&\cdot&\cdot&\cdot\\ \cdot&[illegible]&\cdot&\cdot&\cdot&\cdot\\ \cdot&\cdot&[illegible]&\frac{3k_c}{4}&\cdot&\cdot\\ \cdot&\cdot&\frac{3k_c}{4}&[illegible]&\cdot&\cdot\\ \cdot&\cdot&\cdot&\cdot&[illegible]&\frac{3k_c}{4}\\ \cdot&\cdot&\cdot&\cdot&\frac{3k_c}{4}&[illegible] \end{pmatrix}$$

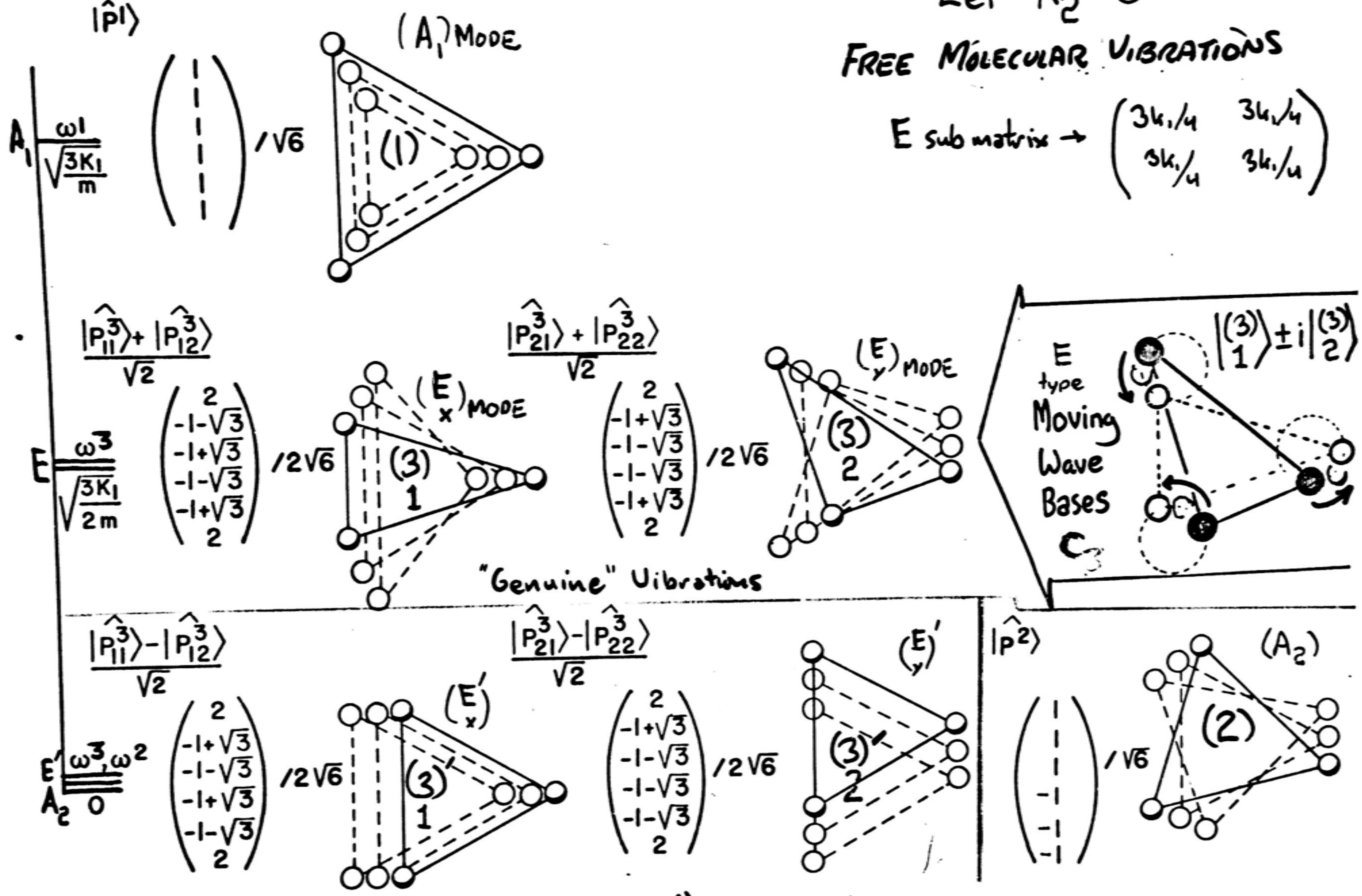
Scanned by CamScanner

3-10

Let $k_2 = 0$

FREE MOLECULAR VIBRATIONS

$$E \text{ submatrix} \rightarrow \begin{pmatrix} 3k_1/4 & 3k_1/4 \\ 3k_1/4 & 3k_1/4 \end{pmatrix}$$



"Non-Genuine" Molecular Vibrations

Scanned by CamScanner

Part 4. Application of Class Algebra

IR CHARACTERS: $\chi^{\alpha}(g) \equiv \mathrm{TRACE}\,\mathcal{D}^{\alpha}(g) = \sum_{i=1}^{\ell^{\alpha}} \mathcal{D}^{\alpha}_{ii}(g) = \chi^{\alpha}(g')$

$\chi(1) = \ell^{\alpha}$ (if: $t g t^{-1} = g'$)

All-commuting idempotents: $\mathbb{P}^{\alpha} = \sum_{i=1}^{\ell^{\alpha}} P^{\alpha}_{ii}$

$$= \sum_{i=1} \sum_{g} (\ell^{\alpha}/{}^{\circ}\mathcal{G})\, \mathcal{D}^{\alpha *}_{ii}(g)\, g$$

"Ab Initio" Derivation of χ^{α}: We use minimal equations $c^n + a c^{n-1} + \ldots + 1 = 0$ of class-sums: $c_g = g + g' + \ldots$

$$\mathbb{P}^{\alpha} = \underbrace{\sum_{g} (\ell^{\alpha}/{}^{\circ}\mathcal{G})\, \chi^{\alpha *}(g)}_{d^{\alpha}_{g}}\, g$$

(define a coefficient)

to derive: $\mathbb{P}^{\alpha} = d^{\alpha}_{1} 1 + d^{\alpha}_{g} c_g + \ldots$

$\mathbb{P}^{\beta} = d^{\beta}_{1} 1 + d^{\beta}_{g} c_g + \ldots$

$\vdots$

then obtain ℓ^{α} from: $d^{\alpha}_{1} = \dfrac{\ell^{\alpha} \chi^{\alpha}(1)^{*}}{{}^{\circ}\mathcal{G}} = \dfrac{(\ell^{\alpha})^2}{{}^{\circ}\mathcal{G}}$

$$\boxed{\ell^{\alpha} = (d^{\alpha}_{1}\, {}^{\circ}\mathcal{G})^{1/2}}$$

...obtain $\chi^{\alpha}(g)$ from: $d^{\alpha}_{g} = \dfrac{\ell^{\alpha} \chi^{\alpha}(g)^{*}}{{}^{\circ}\mathcal{G}}$

$$\boxed{\chi^{\alpha}_{g} = \frac{d^{\alpha *}_{g}\, {}^{\circ}\mathcal{G}}{\ell^{\alpha}}}$$

dim. of ... rank $= \sum \ell_{\alpha}$ (here $= 4$)

Theory and Application of Characters

Suppose you're given a reducible representation...

$$\ldots R(g) = \begin{pmatrix} 1 & \cdots & 1 & & 1 \\ & & & & -1 \\ & & & & \vdots \\ \vdots & & & & \\ 1 & & & & \end{pmatrix}, \quad R(g') = \begin{pmatrix} 1 & \cdots \\ \vdots & \\ \cdots & \end{pmatrix}$$

$R(1) = (\ldots)$, $R(\sigma_1) = (\ldots)$, $R(r) = (\ldots)$, $R(\sigma_2) = (\ldots)$, $R(r^2) = (\ldots)$, $R(\sigma_3) = (\ldots)$

...and want to predict how it will reduce...

$$\ldots \mathcal{T}^{\dagger} R(g) \mathcal{T} = \begin{pmatrix} (\mathcal{D}^{\alpha}_{(g)}) & & \\ 0 & (\mathcal{D}^{\alpha}_{(g)}) & \\ 0 & 0 & (\mathcal{D}^{\beta}_{(g)}) \end{pmatrix}$$

f^{α} blocks

f^{β} blocks

f^{α} is FREQUENCY (no. of times irrep $\mathcal{D}^{\alpha}$ appears)

Let: $g = \mathbb{P}^{\alpha} = \sum_{g} (\ell^{\alpha}/{}^{\circ}\mathcal{G})\, \chi^{\alpha *}_{(g)}\, g = \sum_{\text{classes } j} (\ell^{\alpha}/{}^{\circ}\mathcal{G})\, \chi^{\alpha *}_{j}\, c_j$

$$\mathcal{T}^{\dagger} R(\mathbb{P}^{\alpha}) \mathcal{T} = \begin{pmatrix} 1 & & & & & \\ & 1 & & & & \\ & & 1 & & & \\ & & & 1 & & \\ & & & & 0 & \\ & & & & & 0 \end{pmatrix}$$

$f^{\alpha} = 1/\ell^{\alpha}\, \mathrm{TRACE}\, R(\mathbb{P}^{\alpha})$

$= (1/{}^{\circ}\mathcal{G}) \sum_{j} \chi^{\alpha *}_{j}\, \mathrm{TRACE}\, R(c_j)$

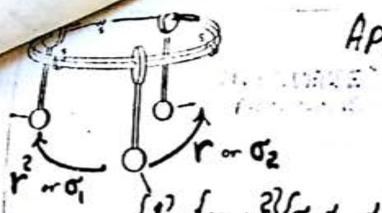
$f^{\alpha} = (1/{}^{\circ}\mathcal{G}) \sum_{j} \chi^{\alpha *}_{j}\, {}^{\circ}c_j\, \mathrm{TRACE}\, R(g_j)$

irrep. character; order of class j; Trace for any element in class j

$\mathrm{TRACE}\, R(\mathbb{P}^{\alpha}) = f^{\alpha} \cdot \ell^{\alpha}$

Scanned by CamScanner

APPLICATION OF CHARACTERS (A) Deriving f^α



$$\{1\}\ \{r, r^2\}\ \{\sigma_1, \sigma_2, \sigma_3\}$$

	$\{1\}$	$\{r, r^2\}$	$\{\sigma_1,\sigma_2,\sigma_3\}$
$\chi^{(1)}=\chi^{A_1}$	1	1	1
$\chi^{(2)}\equiv\chi^{A_2}$	1	1	-1
$\chi^{(3)}\equiv\chi^{E}$	2	-1	0

$$\left\{\begin{pmatrix}1&\cdot&\cdot\\\cdot&1&\cdot\\\cdot&\cdot&1\end{pmatrix},\begin{pmatrix}\cdot&\cdot&1\\1&\cdot&\cdot\\\cdot&1&\cdot\end{pmatrix},\begin{pmatrix}\cdot&1&\cdot\\\cdot&\cdot&1\\1&\cdot&\cdot\end{pmatrix},\begin{pmatrix}1&\cdot&\cdot\\\cdot&\cdot&1\\\cdot&1&\cdot\end{pmatrix},\begin{pmatrix}\cdot&\cdot&1\\\cdot&1&\cdot\\1&\cdot&\cdot\end{pmatrix},\begin{pmatrix}\cdot&1&\cdot\\1&\cdot&\cdot\\\cdot&\cdot&1\end{pmatrix}\right\}$$

$$R(1),\ \underbrace{R(r),\ R(r^2)},\ \underbrace{R(\sigma_3),\ R(\sigma_1),\ R(\sigma_2)}$$

$$\mathrm{TRACE}\,R(1)=3,\quad \mathrm{TRACE}\,R(r)=0,\quad \mathrm{TRACE}\,R(\sigma)=1.$$

$$\boxed{f^\alpha = {}^1\!/{}^\circ G \sum_j \chi_j^{\alpha *}\, {}^\circ c_j\ \mathrm{TRACE}\,R(g_j)}$$

$$f^{(1)} = {}^1\!/_6\left[\chi_1^{(1)*}\,{}^\circ c_1\ \mathrm{TRACE}\,R(1) + \chi_2^{(1)*}\,{}^\circ c_2\ \mathrm{TRACE}\,R(r) + \chi_3^{(1)*}\,{}^\circ c_3\ \mathrm{TRACE}\,R(\sigma)\right]$$

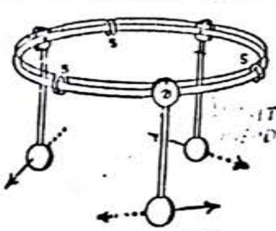
$$f^{A_1}\equiv f^{(1)} = {}^1\!/_6[\,1\cdot 1\cdot 3 + 1\cdot 2\cdot 0 + 1\cdot 3\cdot 1\,] = 1$$

$$f^{(2)} = {}^1\!/_6[\,1\cdot 1\cdot 3 + 1\cdot 2\cdot 0 - 1\cdot 3\cdot 1\,] = 0$$

$$f^{E}\equiv f^{(3)} = {}^1\!/_6[\,2\cdot 1\cdot 3 - 1\cdot 2\cdot 0 + 0\cdot 3\cdot 1\,] = 1$$

$$T^\dagger R(g)\, T = \begin{pmatrix}\boxed{\mathcal{D}^{A_1}_{(g)}} & 0 & 0\\ 0 & \multicolumn{2}{c}{\boxed{\mathcal{D}^{E}_{(g)}}}\\ 0 & & \end{pmatrix}$$

$$T_R^\dagger R\, T_R = A_1 \oplus E$$



$$-|\sigma_3\rangle = |1\rangle$$

$$\begin{pmatrix}1&\cdot&\cdot\\\cdot&1&\cdot\\\cdot&\cdot&1\end{pmatrix}\underbrace{\begin{pmatrix}\cdot&\cdot&1\\1&\cdot&\cdot\\\cdot&1&\cdot\end{pmatrix}\begin{pmatrix}\cdot&1&\cdot\\\cdot&\cdot&1\\1&\cdot&\cdot\end{pmatrix}}\ \underbrace{\begin{pmatrix}-1&\cdot&\cdot\\\cdot&\cdot&-1\\\cdot&-1&\cdot\end{pmatrix}\begin{pmatrix}\cdot&\cdot&-1\\\cdot&-1&\cdot\\-1&\cdot&\cdot\end{pmatrix}\begin{pmatrix}\cdot&-1&\cdot\\-1&\cdot&\cdot\\\cdot&\cdot&-1\end{pmatrix}}$$

$$\mathrm{TRACE}\,S(1)=3,\quad \mathrm{TRACE}\,S(r)=0,\quad \mathrm{TRACE}\,S(\sigma)=-1.$$

$$f^{(1)} = {}^1\!/_6[3+0-3]=0$$

$$f^{A_2}\equiv f^{(2)} = {}^1\!/_6[3+0+3]=1$$

$$f^{E}\equiv f^{(3)} = {}^1\!/_6[6+0-0]=1$$

$$T_S^\dagger S\, T_S = A_2 \oplus E$$

APPLICATION OF CHARACTERS (B.) Deriving Eigenvalues a^α

C_{3v} Three Pendulum problem again:

$$\langle a\rangle = \begin{pmatrix}\langle 1|a|1\rangle & \langle 1|a|r\rangle & \langle 1|a|r^2\rangle\\ \cdot&\cdot&\cdot\\ \cdot&\cdot&\cdot\end{pmatrix} = \begin{pmatrix}2a+b & -a & -a\\ \cdot&\cdot&\cdot\\ \cdot&\cdot&\cdot\end{pmatrix}$$

Single Eigenvalue $a^\alpha = (1/\ell^\alpha)\,\mathrm{Trace}\langle a P^\alpha\rangle = (1/{}^\circ G)\sum_{g\in G}\chi^{\alpha *}_{(g)}\,\mathrm{Trace}\langle a g\rangle$

$$\mathrm{Trace}\langle ag\rangle = \mathrm{Trace}\langle t a g t^{-1}\rangle = \mathrm{Trace}\langle a t g t^{-1}\rangle \quad \text{if } t\in G$$

$$= \mathrm{Trace}\langle a g'\rangle \quad \text{for all } g' \text{ in class of } g$$

So:

$$\boxed{a^\alpha = (1/{}^\circ G)\sum_{\text{classes}}\chi_g^{\alpha *}\,{}^\circ c_g\,\mathrm{Trace}\langle a g\rangle \quad \text{If Irrep } (\alpha) \text{ appears no more than once}}$$

Pendulum Example

$$\mathrm{Trace}\langle ag\rangle = \langle 1|ag|1\rangle + \langle r|ag|r\rangle + \langle r^2|ag|r^2\rangle$$

$$= \langle 1|ag|1\rangle + \langle 1|r^{-1}ag\,r|1\rangle + \langle 1|r^{-2}ag\,r^2|1\rangle$$

$$= \langle 1|a|g\rangle + \langle 1|a|r^{-1}gr\rangle + \langle 1|a|r^{-2}gr^2\rangle$$

$$\mathrm{Trace}\langle a\rangle = \langle 1|a|1\rangle + \langle 1|a|1\rangle + \langle 1|a|1\rangle = 3\langle 1|a|1\rangle = 3(2a+b)$$

$$\mathrm{Trace}\langle ar\rangle = \langle 1|a|r\rangle + \langle 1|a|r\rangle + \langle 1|a|r\rangle = 3\langle 1|a|r\rangle = -3a$$

$$\mathrm{Trace}\langle a\sigma_3\rangle = \langle 1|a|1\rangle + \langle 1|a|r^2\rangle + \langle 1|a|r\rangle = b$$

$$a^{A_1} = (1/6)\,[\,1\cdot 3(2a+b) + 1\cdot 2(-3a) + 1\cdot 3\cdot(b)\,] = b$$

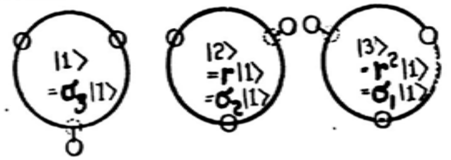
$$a^{E} = (1/6)\,[\,2\cdot 3(2a+b) - 1\cdot 2(-3a) + 0\,] = 3a+b$$

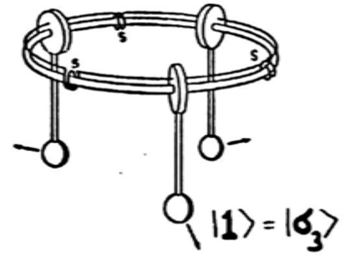
$$a^{A_2} = 0$$

"Transverse" C_{3v} Pendulums

(Solved by P_{ij}^{α} operators)

Base States:



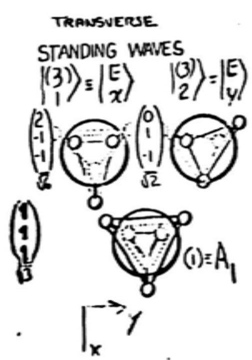


$$R(1)=\begin{pmatrix}1&\cdot&\cdot\\\cdot&1&\cdot\\\cdot&\cdot&1\end{pmatrix}\quad R(r)=\begin{pmatrix}\cdot&\cdot&1\\1&\cdot&\cdot\\\cdot&1&\cdot\end{pmatrix}\quad R(r^2)=\begin{pmatrix}\cdot&1&\cdot\\\cdot&\cdot&1\\1&\cdot&\cdot\end{pmatrix}\quad R(\sigma_1)=\begin{pmatrix}\cdot&\cdot&1\\\cdot&1&\cdot\\1&\cdot&\cdot\end{pmatrix}\quad R(\sigma_2)=\begin{pmatrix}\cdot&1&\cdot\\1&\cdot&\cdot\\\cdot&\cdot&1\end{pmatrix}\quad R(\sigma_3)=\begin{pmatrix}1&\cdot&\cdot\\\cdot&\cdot&1\\\cdot&1&\cdot\end{pmatrix}$$

$$R(P^{(1)})=\begin{pmatrix}1/3&&\\1/3&&\\1/3&&\end{pmatrix}\quad R(P^{(2)})=\begin{pmatrix}0&&\\0&&\\0&&\end{pmatrix}\quad R(P^{(3)}_{11})=\begin{pmatrix}2/3&&\\-1/3&&\\-1/3&&\end{pmatrix}\quad R(P_{12})=\begin{pmatrix}0&&\\0&&\\0&&\end{pmatrix}\quad R(P_{21})=\begin{pmatrix}0&&\\\sqrt{3}/3&&\\-\sqrt{3}/3&&\end{pmatrix}\quad R(P_{22})=\begin{pmatrix}0&0&0\\0&1/2&-1/2\\0&-1/2&1/2\end{pmatrix}$$

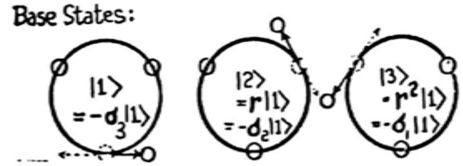
$$\begin{pmatrix}1/\sqrt{3}&1/\sqrt{3}&1/\sqrt{3}\\\sqrt{\frac{2}{3}}&-\frac{1}{2}\sqrt{\frac{2}{3}}&-\frac{1}{2}\sqrt{\frac{2}{3}}\\0&1/\sqrt{2}&-1/\sqrt{2}\end{pmatrix}\begin{pmatrix}\text{representation}\\R(g)\end{pmatrix}\begin{pmatrix}1/\sqrt{3}&\sqrt{\frac{2}{3}}&0\\1/\sqrt{3}&-\frac{1}{2}\sqrt{\frac{2}{3}}&1/\sqrt{2}\\1/\sqrt{3}&-\frac{1}{2}\sqrt{\frac{2}{3}}&-1/\sqrt{2}\end{pmatrix}=\begin{pmatrix}\mathcal{D}^{(1)}(g)&\cdot&\cdot\\\cdot&\mathcal{D}^{(3)}_{11}(g)&\mathcal{D}_{12}\\\cdot&\mathcal{D}_{21}&\mathcal{D}_{22}\end{pmatrix}$$

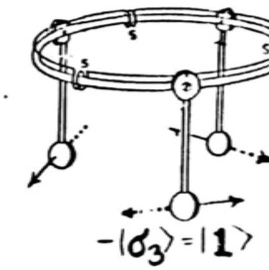
$$\begin{pmatrix}1/\sqrt{3}&1/\sqrt{3}&1/\sqrt{3}\\2/\sqrt{6}&-1/\sqrt{6}&-1/\sqrt{6}\\0&1/\sqrt{2}&-1/\sqrt{2}\end{pmatrix}\begin{pmatrix}\text{acceleration}\\\text{matrix}\\\langle a\rangle\end{pmatrix}\begin{pmatrix}1/\sqrt{3}&2/\sqrt{6}&0\\1/\sqrt{3}&-1/\sqrt{6}&1/\sqrt{2}\\1/\sqrt{3}&-1/\sqrt{6}&-1/\sqrt{2}\end{pmatrix}=\begin{pmatrix}a^{(1)}&\cdot&\cdot\\\cdot&a^{(3)}&0\\\cdot&0&a^{(3)}\end{pmatrix}$$



"Longitudinal" C_{3v} Pendulums

Base States:



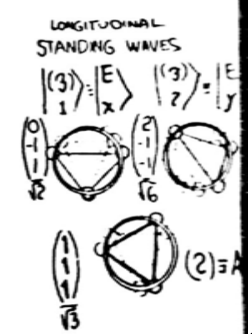


$$\mathcal{S}(1)=\begin{pmatrix}1&\cdot&\cdot\\\cdot&1&\cdot\\\cdot&\cdot&1\end{pmatrix}\quad \mathcal{S}(r)=\begin{pmatrix}\cdot&\cdot&1\\1&\cdot&\cdot\\\cdot&1&\cdot\end{pmatrix}\quad \mathcal{S}(r^2)=\begin{pmatrix}\cdot&1&\cdot\\\cdot&\cdot&1\\1&\cdot&\cdot\end{pmatrix}\quad \mathcal{S}(\sigma_1)=\begin{pmatrix}\cdot&\cdot&-1\\&-1&\cdot\\-1&\cdot&\cdot\end{pmatrix}\quad \mathcal{S}(\sigma_2)=\begin{pmatrix}&-1&\cdot\\-1&\cdot&\cdot\\\cdot&\cdot&-1\end{pmatrix}\quad \mathcal{S}(\sigma_3)=\begin{pmatrix}-1&&\\\cdot&&-1\\\cdot&-1&\cdot\end{pmatrix}$$

$$\mathcal{S}(P^{(1)})=\begin{pmatrix}0&&\\0&&\\0&&\end{pmatrix}\quad \mathcal{S}(P^{(2)})=\begin{pmatrix}1/3&&\\1/3&&\\1/3&&\end{pmatrix}\quad \mathcal{S}(P^{(3)}_{11})=\begin{pmatrix}0&&\\0&&\\0&&\end{pmatrix}\quad \mathcal{S}(P_{12})=\begin{pmatrix}0&&\\-\sqrt{3}/3&&\\\sqrt{3}/3&&\end{pmatrix}\quad \mathcal{S}(P_{21})=\begin{pmatrix}0&&\\0&&\\0&&\end{pmatrix}\quad \mathcal{S}(P_{22})=\begin{pmatrix}2/3&&\\-1/3&&\\-1/3&&\end{pmatrix}$$

$$\begin{pmatrix}1/\sqrt{3}&1/\sqrt{3}&1/\sqrt{3}\\0&-1/\sqrt{2}&1/\sqrt{2}\\2/\sqrt{6}&-1/\sqrt{6}&-1/\sqrt{6}\end{pmatrix}\begin{pmatrix}\text{representation}\\\mathcal{S}(g)\end{pmatrix}\begin{pmatrix}1/\sqrt{3}&0&2/\sqrt{6}\\1/\sqrt{3}&-1/\sqrt{2}&-1/\sqrt{6}\\1/\sqrt{3}&1/\sqrt{2}&-1/\sqrt{6}\end{pmatrix}=\begin{pmatrix}\mathcal{D}^{(2)}(g)&\cdot&\cdot\\\cdot&\mathcal{D}^{(3)}_{11}(g)&\mathcal{D}_{12}\\\cdot&\mathcal{D}_{21}&\mathcal{D}_{22}\end{pmatrix}$$

$$\begin{pmatrix}1/\sqrt{3}&1/\sqrt{3}&1/\sqrt{3}\\0&-1/\sqrt{2}&1/\sqrt{2}\\2/\sqrt{6}&-1/\sqrt{6}&-1/\sqrt{6}\end{pmatrix}\begin{pmatrix}\text{acceleration}\\\text{matrix}\\\langle a\rangle\end{pmatrix}\begin{pmatrix}1/\sqrt{3}&0&2/\sqrt{6}\\1/\sqrt{3}&-1/\sqrt{2}&-1/\sqrt{6}\\1/\sqrt{3}&1/\sqrt{2}&-1/\sqrt{6}\end{pmatrix}=\begin{pmatrix}a^{(2)}&&\\&a^{(3)}&0\\&0&a^{(3)}\end{pmatrix}$$



Scanned by CamScanner

$$\ell^{\alpha} = \left(d_1^{\alpha}\ {}^{\circ}g\right)^{1/2} \qquad \ell^{A_1} = \frac{n!}{\boxed{4\,|\,2\,|\,1\,|\,1}} = 3 \qquad \ell^{E} = \frac{4\cdot 3\cdot 2\cdot 1}{\boxed{\begin{smallmatrix}3 & 2\\ 2 & 1\end{smallmatrix}}} = 2$$

Class Algebra for Octahedral O Group

$$\mathbf{c}_4^2 = 6\mathbf{1} + 3\mathbf{c}_1 + 2\mathbf{c}_2 \dashrightarrow \mathbf{c}_4^3 = 6\mathbf{c}_4 + 3\mathbf{c}_1\mathbf{c}_4 + 2\mathbf{c}_2\mathbf{c}_4$$

$$= 6\mathbf{c}_4 + 12\mathbf{c}_3 + 12\mathbf{c}_4 + 4\mathbf{c}_3 + 2\mathbf{c}_4$$

$$\mathbf{c}_4^3 = 20\mathbf{c}_4 + 16\mathbf{c}_3 \rightarrow \mathbf{c}_4^4 = 20\mathbf{c}_4 + 16\mathbf{c}_3\mathbf{c}_4$$

$$= 20\mathbf{c}_4^2 + 16(3\mathbf{c}_1 + 4\mathbf{c}_2)$$

$$\mathbf{c}_4^4 = 20\mathbf{c}_4^2 + 64\mathbf{c}_2 + 48\mathbf{c}_1 \rightarrow \mathbf{c}_4^5 = 20\mathbf{c}_4^3 + 64\mathbf{c}_2\mathbf{c}_4 + 48\mathbf{c}_1\mathbf{c}_4$$

$$= 20\mathbf{c}_4^3 + 64(2\mathbf{c}_3 + \mathbf{c}_4) + 48(4\mathbf{c}_3 + 4\mathbf{c}_4)$$

$$\mathbf{c}_4^5 = 20\mathbf{c}_4^3 + 256\mathbf{c}_4 + 320\mathbf{c}_3$$

$$\mathbf{c}_4^5 = 40\mathbf{c}_4^3 - 144\mathbf{c}_4$$

$$(c_4^4 - 40c_4^2 + 144)c_4 = 0$$

$$(c_4^2 - 4)\,c_4\,(c_4^2 - 36) = 0$$

$$c_4 = +\underline{2}, -\underline{2}, \underline{0}, +\underline{6}, -\underline{6}.$$

$$\mathbb{P}^{A_1} = \tfrac{1}{24}[\mathbf{1} + \mathbf{c}_1 + \mathbf{c}_2 + \mathbf{c}_3 + \mathbf{c}_4]$$

$$\mathbb{P}^{A_2} = \tfrac{1}{24}[\mathbf{1} + \mathbf{c}_1 + \mathbf{c}_2 - \mathbf{c}_3 - \mathbf{c}_4]$$

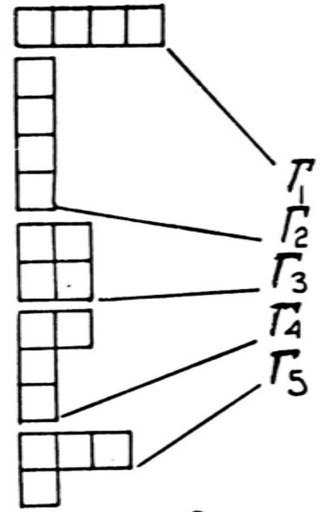
$$\mathbb{P}^{E} = \tfrac{1}{12}[2\mathbf{1} - \mathbf{c}_1 + 2\mathbf{c}_2]$$

$$\mathbb{P}^{T_1} = \tfrac{1}{8}\cancel{\tfrac{3}{}}[3\mathbf{1} \quad - \mathbf{c}_2 - \mathbf{c}_3 + \mathbf{c}_4]$$

$$\mathbb{P}^{T_2} = \tfrac{1}{8}\cancel{\tfrac{3}{}}[3\mathbf{1} \quad - \mathbf{c}_2 + \mathbf{c}_3 - \mathbf{c}_4]$$

j	1	c.r	R²	R	c.i
$\chi_j^{A_1}$	1	1	1	1	1
$\chi_j^{A_2}$	1	1	1	-1	-1
χ_j^{E}	2	-1	2	0	0
$\chi_j^{T_1}$	3	0	-1	+1	-1
$\chi_j^{T_2}$	3	0	-1	-1	+1

18.3

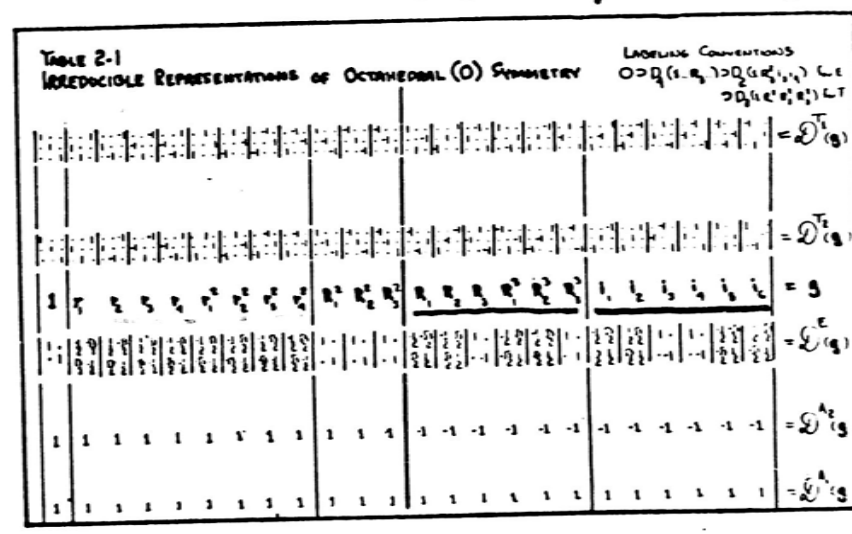


Permutation Grp. S_4
Tableau Labeling

O Characters

		[111]	[100]		[110]	axes
	0°	120°	180°	90°	180°	angle
Γ_1 A_1	1	1	1	1	1	
Γ_2 A_2	1	1	1	-1	-1	
Γ_3 E	2	-1	2	0	0	
Γ_4 T_1	3	0	-1	+1	-1	
Γ_5 T_2	3	0	-1	-1	+1	

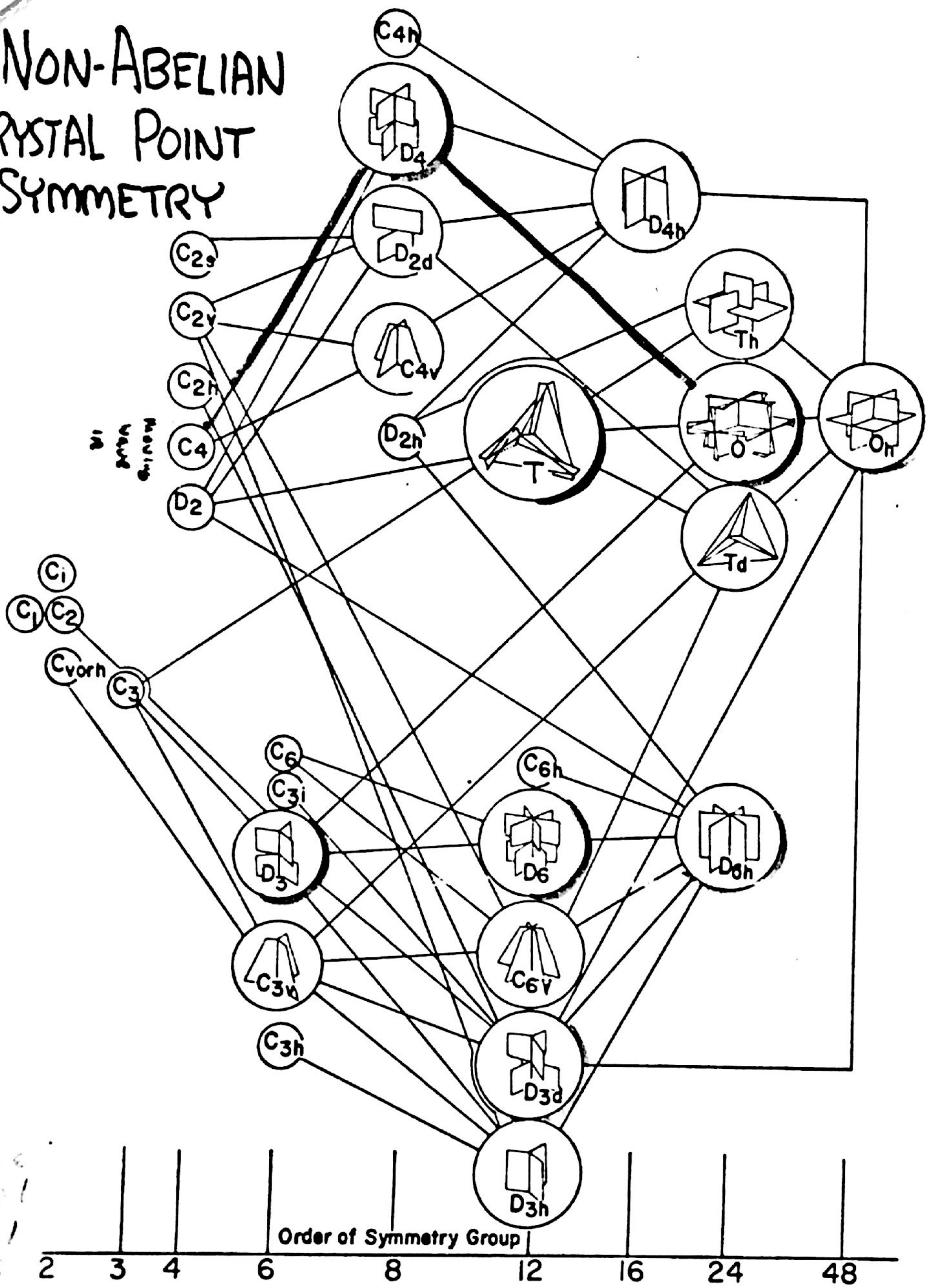
O Irr. Reps. (tetragonal..



17-10

Scanned by CamScanner

NON-ABELIAN CRYSTAL POINT SYMMETRY



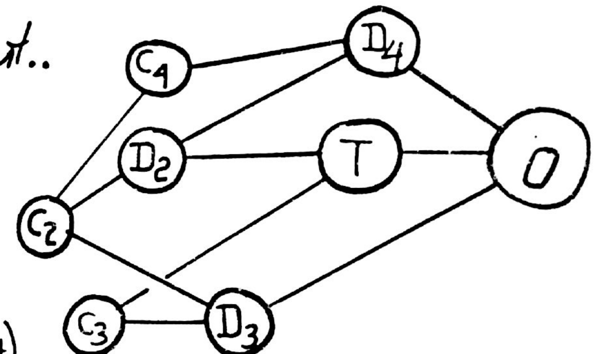
Q. How does one split $\mathbb{P}^E$, $\mathbb{P}^{T_1}$, or $\mathbb{P}^{T_2}$ into irreducible idempotents? i.e.: $\mathbb{P}^E = P^E_{11} + P^E_{22}$, $\mathbb{P}^{T_1} = P^{T_1}_{11} + P^{T_1}_{22} + P^{T_1}_{33}$

($\mathbb{P}^{A_1}$ and $\mathbb{P}^{A_2}$ won't split anymore..) $\mathbb{P}^{T_2} = P^{T_2}_{11} + P^{T_2}_{22} + P^{T_2}_{33}$

A. Use subgroup idempotents

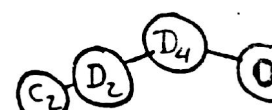
Q. Which subgroups?

A. Many choices... pick whichever is convenient..

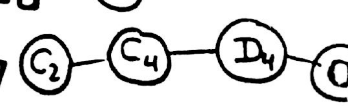


... each chain may correspond to a different (but equivalent) set of irreps ...

Case 1. TETRAGONAL STANDING WAVE CHOICE $C_2 \subset D_2 \subset D_4 \subset O$



Case 2. " MOVING " $C_2 \subset C_4 \subset D_4 \subset O$



Case 3. TRIGONAL STANDING WAVE CHOICE $C_2 \subset D_3 \subset O$

Scanned by CamScanner