

Relations among representations of groups and their subgroups (40)

1) from a group G to its subgroup H or restriction

- if we restrict a certain representation Γ of the group G only to elements of its subgroup H , we get again a representation but this time of the subgroup H
- such a representation is called a restricted representation

$\Gamma \downarrow H$ from G to H

- if Γ is one of IRs of G , i.e. Γ_G^M with $\chi_G^M(g)$,

then $\Gamma_G^M \downarrow H$ is, in general, a reducible repr. of H

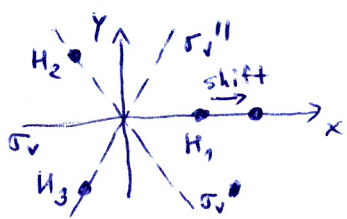
with the character $\chi_H^{M \downarrow H}(h) = \chi_G^M(h)$ for all $h \in H$

and we can decompose it into IRs of H using the formula

$$\alpha_\nu^{M \downarrow H} = \frac{1}{\#H} \sum_{h \in H} \chi_H^\nu(h)^* \chi_G^M(h)$$

where $\alpha_\nu^{M \downarrow H}$ denotes the number how many times the IR Γ_H^ν is contained in the restricted repr. $\Gamma_G^M \downarrow H$.

Examples: a) restriction from C_{3v} onto a subgroup $H = \{E, \sigma_v\} \sim C_s$



when the symmetry of the molecule NH_3 (ammonia) is broken by prolongation of one of the N-H bonds

- using the character tables we find

C_{3v}	E	$2C_3$	$3\sigma_v$
A_1	1	1	1
A_2	1	1	-1
E	2	-1	0

$H \sim C_s$	E	σ_v
A'	1	1
A''	1	-1

characters of IRs of $H \sim C_s$

$A' = A_1 \downarrow H$	1	1
$A'' = A_2 \downarrow H$	1	-1
$A' \oplus A'' = E \downarrow H$	2	0

characters of restricted representations

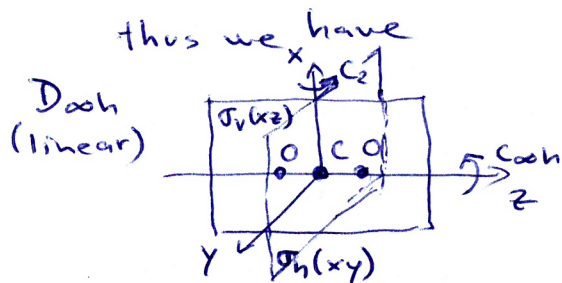
decomposition either by using the formula for $\alpha_\nu^{M \downarrow H}$, for example $\alpha_{A'}^{E \downarrow H} = \frac{1}{2}(1 \cdot 2 + 1 \cdot 0) = 1$ etc.

or simply by looking at IRs of $H \sim C_s$ and adding them up to get $E \downarrow H$

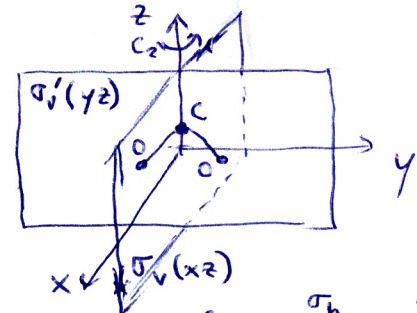
- we see that doubly generated states belonging to E will become two non-generate states belonging to A' and A''

b) restriction from $D_{\infty h}$ (linear geometry) to C_{2v} (bend geometry) (41)

- it describes what happens with states of CO_2 molecule when the symmetry is broken by bending
- it is necessary to be careful with the orientation of coordinate systems
- usual orientation is that the z -axis is the main rotational axis which is different for $O=C=O \rightarrow z$ and for $O=C=O$



C_{2v} (bend)



- standard character tables

$D_{\infty h}$	E	$2C_{\infty}(\phi)$	$\dots$	$C_2(z)$	$\infty\sigma_v$	$\sigma_h(xy)$	$2S_{\infty}(\phi)$	$\dots$	i	∞C_2	C_{2v}	E	$C_2(z)$	$\sigma_v(xz)$	$\sigma_v'(yz)$	
Σ_g^+	1	1	$\dots$	1	1	1	1	$\dots$	1	1	A_1	1	1	1	1	z
$R_z \rightarrow \Sigma_g^-$	1	1	$\dots$	1	-1	1	1	$\dots$	1	-1	A_2	1	1	-1	-1	R_z
$(R_x, R_y) \rightarrow \Pi_g$	2	$2\cos\phi$	$\dots$	-2	0	-2	$-2\cos\phi$	$\dots$	2	0	B_1	1	-1	1	-1	x, R_y
Δ_g	2	$2\cos 2\phi$	$\dots$	2	0	2	$2\cos 2\phi$	$\dots$	2	0	B_2	1	-1	-1	1	y, R_x
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\Sigma_g^- \downarrow C_{2v}$	1	-1	1	-1	$= B_1$
$z \rightarrow \Sigma_u^+$	1	1	$\dots$	1	1	-1	-1	$\dots$	-1	-1	$\Pi_g \downarrow C_{2v}$	2	0	-2	0	$= A_1 \oplus B_2$
Σ_u^-	1	1	$\dots$	1	-1	1	1	$\dots$	1	-1	$\Sigma_u^+ \downarrow C_{2v}$	1	-1	-1	1	$= B_2$
$(x, y) \rightarrow \Pi_u$	2	$2\cos\phi$	$\dots$	-2	0	2	$2\cos\phi$	$\dots$	-2	0	$\Pi_u \downarrow C_{2v}$	2	0	2	0	$= A_1 \oplus B_1$
Δ_u	2	$2\cos 2\phi$	$\dots$	2	0	-2	$-2\cos 2\phi$	$\dots$	-2	0						

- ! assignment of x, y, z and R_x, R_y, R_z to IRs of $D_{\infty h}$ and C_{2v} can be confusing, it is not true in our case that $\Pi_u = B_1 \oplus B_2$
- to decompose the restricted repr. correctly

it is necessary to use the following correspondence

in $D_{\infty h}$: $x \leftrightarrow z$ in C_{2v} } $\Rightarrow \Pi_u = A_1 \oplus B_1$ better to write $\Pi_u \downarrow C_{2v} = A_1 \oplus B_1$ etc.

$y \leftrightarrow x$

$z \leftrightarrow y$ $\Rightarrow \Sigma_u^+ = B_2$

$R_x \leftrightarrow R_z$ } $\Rightarrow \Pi_g = A_2 \oplus B_2$

$R_y \leftrightarrow R_x$ } $\Rightarrow \Pi_g = A_2 \oplus B_2$

$R_z \leftrightarrow R_y$ $\Rightarrow \Sigma_g^- = B_1$

in agreement with decompositions below the character table for C_{2v}

2) Induction from a subgroup to the group

- this is more complicated than restriction, but doable.

- let G be a group and H its subgroup

then G can be decomposed to left cosets $G = g_1^e H + g_2 H + \dots + g_M H$

where g_i can be chosen arbitrarily from the left cosets and $M = \frac{\#G}{\#H}$

- let $D_H(h)$ be an arbitrary matrix repr. of the subgroup H

and let $\phi_1, \dots, \phi_d$ be a basis of this repr. - it is a basis of some invariant irred. subspace under H -action, but not necessarily under G

that is we have $T(h) \phi_i = \sum_{j=1}^d \phi_j D_H(h)_{ji}$ for all $h \in H$

- let us define formally (we assume that in this way we get linearly independent functions)

$\phi_{ti} = T(g_t) \phi_i$ where g_t define left cosets of H in G , $t=1, \dots, M$, $i=1, \dots, d$

and show that these functions form a basis of $M \times d$ -dimensional repr. of G , i.e., they satisfy

$$T(g) \phi_{ti} = \sum_{sj} \phi_{sj} D_G(g)_{sj, ti}$$

- by the action of g we get

$$\begin{aligned} T(g) \phi_{ti} &= T(g g_t) \phi_i = T(g_s) T(g_s^{-1} g g_t) \phi_i = \uparrow \text{ here we use that } \\ &= T(g_s) \sum_{j=1}^d \phi_j D_H(g_s^{-1} g g_t)_{ji} = \text{ } g g_t \text{ belongs to some } \\ &= \sum_j \phi_{sj} D_H(g_s^{-1} g g_t)_{ji} \text{ left coset, e.g. } g_s H \\ & \text{ and we have } g_s^{-1} g g_t \in H \end{aligned}$$

and thus $T(g) \phi_{ti}$ is a linear combination of ϕ_{sj} and

moreover, for such s that $g g_t \in g_s H$, therefore, the matrix

$D_G(g)$ can be obtained by adding $\delta_{st}(g) = \begin{cases} 1 & \text{for } g g_t \in g_s H \\ 0 & \text{otherwise} \end{cases}$

or
$$D_G(g)_{sj, ti} = \delta_{st}(g) D_H(g_s^{-1} g g_t)_{ji}$$

this is the induced representation of G from the repr. $D_H(h)$

of H denoted by $D_G = D_H \uparrow G$

- we can easily check that it is really repr. of G :

a) for $g=e$ we get $g_t = g_s \Rightarrow D_G(e) = \mathbb{1}_{M \times M}$

$$\begin{aligned}
 b) \quad D_G(g) D_G(g') &\Leftrightarrow \sum_{r,k} D_G(g)_{sj,rk} D_G(g')_{rk,ti} = \\
 &= \sum_{r,k} \underbrace{\delta_{sr}(g) \delta_{kt}(g')}_{\substack{1 \text{ for } ggr = gsh \text{ for } h \in H \\ g'g_t = g_rh' \text{ for } h' \in H}} D_H(g_s^{-1} g g_r)_{jk} D_H(g_r^{-1} g' g_t)_{ki} = \\
 &= \delta_{st}(gg') D_H(g_s^{-1} g g' g_t)_{ji} = D_G(gg')_{sj,ti} \Leftrightarrow D_G(gg')
 \end{aligned}$$

- if $D_H(h)$ is unitary then $D_G(g)$ is also unitary

$$\begin{aligned}
 [D_G(g)^{-1}]_{sj,ti} &= \delta_{st}(g') D_H(g_s^{-1} g' g_t)_{ji} \stackrel{\substack{\text{Unitarity of } D_H \\ \downarrow}}{=} \delta_{ts}(g) D_H(g_t^{-1} g g_s)_{ij}^* \\
 &= \delta_{ts}(g) D_H(g_t^{-1} g g_s)_{ij}^* = D_G(g)_{ti,sj}^* = [D_G(g)^{\dagger}]_{sj,ti}
 \end{aligned}$$

$g'g_t = gsh \Rightarrow g g_s = g_t h^{-1}$

- the character of this induced repr. is

$$\boxed{\chi_G(g) = \sum_{s,j} \delta_{ss}(g) D_H(g_s^{-1} g g_s)_{jj} = \sum_s \delta_{ss}(g) \chi_H(g_s^{-1} g g_s)}$$

- induced representations are, in general, reducible, even if we start with an irreducible repr. Γ_H^ν of H , thus we set deco-position

$$\chi^{\nu \uparrow G}(g) = \sum_M \alpha_M^{\nu \uparrow G} \chi_G^M(g)$$

character of the induced repr. from IR Γ_H^ν of H
characters of IRs Γ_G^M of G

which can be also written as

$$\chi^{\nu \uparrow G}(g) = \sum_s \delta_{ss}(g) \chi_H^\nu(g_s^{-1} g g_s) \stackrel{\substack{\text{we divide by } \#H \\ \text{because we can choose } \#H \text{ different } g_s}}{=} \frac{1}{\#H} \sum_{\substack{g'g'g' \in H \\ \text{necessary condition to count only correct terms}}} \chi_H^\nu(g_s^{-1} g g_s)$$

here, we replace the sum over Melen. g_s by the sum over the whole G

(since for any $a \in g_s H$ we get $a = g_s h$
and $a^{-1} g a = h^{-1} g_s^{-1} g g_s h \in H$ if $g_s^{-1} g g_s \in H$)

- thus $\alpha_M^{\nu \uparrow G}$ denotes the number how many times the IR Γ_G^M is contained in the induced repr. $\Gamma_H^\nu \uparrow G$

- $\alpha_M^{\nu \uparrow G}$ is related to $\alpha_\nu^{M \downarrow H}$ for the restricted representations via Frobenius reciprocity theorem

Frobenius reciprocity theorem

(44)

Let $\alpha_M^{\nu \uparrow G}$ denotes the number how many times the IR Γ_G^M of the group G is contained in the induced repr. $\Gamma_H^{\nu \uparrow G}$ from the IR Γ_H^{ν} of its subgroup

and $\alpha_{\nu}^{M \downarrow H}$ denotes the number how many times the IR Γ_H^{ν} of H is contained in the restricted repr. $\Gamma_G^M \downarrow H$ from Γ_G^M of G ,

then $\alpha_M^{\nu \uparrow G} = \alpha_{\nu}^{M \downarrow H}$ for all Γ_G^M and Γ_H^{ν} .

Proof: we have

$$\begin{aligned} \alpha_M^{\nu \uparrow G} &= \frac{1}{\#G} \sum_{g \in G} \chi_G^M(g)^* \chi^{\nu \uparrow G}(g) = \frac{1}{\#G} \sum_{g \in G} \chi_G^M(g)^* \frac{1}{\#H} \sum_{g' \in G} \chi_H^{\nu}(g'^{-1} g g') = \\ &= \frac{1}{\#G} \frac{1}{\#H} \sum_{h \in H} \sum_{g' \in G} \chi_G^M(g' h g'^{-1})^* \chi_H^{\nu}(h) \quad \begin{array}{l} \text{substitution} \\ \text{for } h = g'^{-1} g g' \text{ gives} \\ g = g' h g'^{-1} \end{array} \\ &\quad \begin{array}{l} \text{conjugate element} \\ \text{to } h \rightarrow \text{the same} \\ \text{character as } h \end{array} \\ &= \frac{\sum_{g \in G} 1}{\#G} \frac{1}{\#H} \sum_{h \in H} \chi_G^M(h)^* \chi_H^{\nu}(h) = \alpha_{\nu}^{M \downarrow H} = \frac{1}{\#H} \sum_{h \in H} \chi_H^{\nu}(h)^* \chi_G^M(h) \end{aligned}$$

Basic examples: for trivial subgroups of G we get

1) if $H = G$ then $M=1$, $g_1=e$ and $D_H \uparrow G = D_H$ (the same repr.)

2) if $H = \{e\}$ then $M=\#G$, $gH = \{g\}$ and H has only one IR which is the trivial one $D_H(e) = 1$

and thus, $D_G(g)_{st} = \delta_{st}(g) = \begin{cases} 1 & \text{for } g g t = g s \\ 0 & \text{for } g g t \neq g s \end{cases}$

that is, we set the regular representation

Notes: 1) Notice that from each IR Γ^{ν} of H we can make a repr. of G that has decomp-osition into IRs of G and thus every IR of H must be contained in a certain decomp-osition of $\Gamma_G^M \downarrow H$.

2) And similarly every IR of G must be contained in a certain decomp-osition of $\Gamma_H^{\nu \uparrow G}$.

3) Irreducible representations of a group $G = H_1 \otimes H_2$

(45)

- let us have a group G that is a direct product of its two subgroups H_1 and H_2 , that is we can express any $g \in G$ as a product of $h_1 \in H_1$ and $h_2 \in H_2$: $g = h_1 h_2$

- then from arbitrary $\Gamma_{H_1}^\mu$ and $\Gamma_{H_2}^\nu$ (IRs of H_1 and H_2)

we set IR of G as a direct product of corresponding matrices

$$D_{ke,ij}^{\mu\nu}(g=h_1 h_2) = D_{ki}^\mu(h_1) D_{ej}^\nu(h_2)$$

with the character

$$\chi^{\mu\nu}(g=h_1 h_2) = \chi^\mu(h_1) \chi^\nu(h_2)$$

- we can easily check that this repr. is irreducible using the

Frobenius criterion of irreducibility: $\Gamma_{H_1}^\mu$ and $\Gamma_{H_2}^\nu$ are irreducible

$$\sum_{g \in G} |\chi^{\mu\nu}(g)|^2 \stackrel{g=h_1 h_2}{=} \sum_{h_1 \in H_1} \sum_{h_2 \in H_2} |\chi^\mu(h_1)|^2 |\chi^\nu(h_2)|^2 \stackrel{\downarrow}{=} \#H_1 \cdot \#H_2 = \#G$$

- moreover, in this way, we get all IRs of G , since

$$\sum_{\mu, \nu} (d_\mu d_\nu)^2 = \sum_{\mu} d_\mu^2 \cdot \sum_{\nu} d_\nu^2 = \#H_1 \cdot \#H_2 = \#G$$

where d_μ and d_ν are dimensions of $\Gamma_{H_1}^\mu$ and $\Gamma_{H_2}^\nu$.

Example: group $D_{3h} = C_{3v} \otimes C_s$

where $C_{3v} = \{E, C_3, C_3^2, \sigma_v, \sigma_v', \sigma_v''\}$ and $C_s = \{E, \sigma_h\}$

as $\sigma_h C_{3v} = \{\sigma_h, S_3, S_3^5, C_2, C_2', C_2''\}$

the character table of D_{3h} can be obtained from

C_{3v}	E	$2C_3$	$3\sigma_v$
A_1	1	1	1
A_2	1	1	-1
E	2	-1	0

and

C_s	E	σ_h
A'	1	1
A''	1	-1

by making "a product" of these tables

(C_{3v} table is 3x multiplied by 1 and 1x by -1,

see the table for D_{3h} on page (T9)