

# RELATIONS BETWEEN REPRESENTATIONS OF A GROUP & ITS SUBGROUPS

(56)

## A) SUBDUCED REPRESENTATIONS

Def: Let  $T(g)$  be operators of a repre  $(\rho, V)$  of  $G$  and let  $H \subset G$  is a subgroup. Then

$$\rho_{vH} = \{T(h) / h \in H\}$$

forms subduced representation of  $H$

•  $\rho_{vH}$  in general reducible even for  $\rho$  IRREP of  $G$

$$\rho_{vH} = \bigoplus_{\mu} \chi_{\mu}^{vH} \rho_{vH}^{\mu} \Leftrightarrow \chi_{\mu}^{vH} = \frac{1}{\#H} \sum_{h \in H} X_H^{\mu}(h)^* \chi(h)$$

Example: •  $H = C_3 = \{E, \sigma_v\} \subset G = C_{3v} = \{E, \sigma_v, \sigma_{3v}\}$

$C_{3v}$	$E$	$\sigma_{3v}$	$\sigma_v$	
$A_1$	1	1	1	$\rightarrow A_1 _{vC_3} = A'$
$A_2$	1	1	-1	$\rightarrow A_2 _{vC_3} = A''$
$E$	2	-1	0	$\rightarrow E _{vC_3} = A' \oplus A''$
$C_3$	$E$		$\sigma_v$	
$A'$	1		1	
$A''$	1		-1	

## B) INDUCED REPRESENTATIONS (For finite groups)

• let  $H \subset G$  &  $D_H(h)$  is a cl-dim. repre of  $H$   
 $\Rightarrow$  can we construct a repre of the full  $G$ ?

YES, by explicit construction of its basis!

1, decomposition of  $G$  into left cosets with resp. to  $H$

$$G = p_1 H + p_2 H + \dots + p_M H \quad M = \frac{\# G}{\# H} \quad (\text{Lagrange})$$

- $p_i$ : fixed representatives of individual classes

- $p_1 = e$

2, basis of the induced repres. of  $G$

- Let  $\{\phi_1, \dots, \phi_d\}$  be the basis of  $D_H$

$$\Rightarrow T(h)\phi_i = \sum_{j=1}^d \phi_j D_H(h)_i^j$$

rep. space  
of  $D_H$

$$\text{span}\{\phi_{t,i}\} = \bigoplus_{t=1}^M p_t V_H$$

$\uparrow$   
isomorphic copy of  $V_H$

- def.  $\phi_{t,i} \equiv T(p_t)\phi_i \quad t = 1, \dots, M; i = 1, \dots, d$

(they are abstract objects not living in the rep. space of  $D_H$ , we don't really know what they are...)  
 $\Rightarrow \phi_{t,i}$  forms a basis of  $dM$ -dim. repres. of  $G$ )

(we will not prove they are lin. indep.):

$$T(g)\phi_{t,i} = T(g p_t)\phi_i = T(p_s p_s^{-1} g p_t)\phi_i = T(p_s)T(p_s^{-1} g p_t)\phi_i$$

- $p_s$ :  $p_s^{-1} g p_t \in H \Leftrightarrow g p_t \in p_s H$

(such  $p_s$  exists and is unique because  $g p_t = g' \in G$  and each element of  $G$  belongs to exactly one coset)

$$\Rightarrow T(g)\phi_{t,i} = T(p_s) \sum_j \phi_j D_H(p_s^{-1} g p_t)_i^j = \sum_j \phi_{s,j} D_H(p_s^{-1} g p_t)_i^j$$

for  $g p_t \in p_s H$

- def.  $\delta_{st}(g) = \begin{cases} 1 & g p_t \in p_s H \\ 0 & g p_t \notin p_s H \end{cases}$

$$\Rightarrow D_G(g)_{ti}^{sj} = \delta_{st}(g) D_H(p_s^{-1} g p_t)_i^j$$

induced repres. of  $G$

$$D_G = D_H \rtimes G$$

• note that we don't really know what  $T(p_\epsilon) \phi_i$  is  
but we don't need to in the end... (58)

3,  $D_G(g)_{\epsilon i}^{sj}$  is indeed a replic

$$a, g \in e \Rightarrow \delta_{st}(e) = \delta_{st} : e p_\epsilon = p_\epsilon \in P_\epsilon H$$

$$\Rightarrow D_H(P_s^{-1}g P_\epsilon) = D_H(P_\epsilon^{-1}e P_\epsilon) = D_H(e) = 1$$

$$\Rightarrow D_G(e) = \prod_{\text{dim } \times \text{dim}}$$

this selects one unique  $r$  from the  $\sum_r$

$$\sum_{rk} D_G(g)_{rk}^{sj} D_G(g)_{ti}^{rk} = \sum_{rk} \delta_{sr}(g) \delta_{rt}(g) D_H(P_s^{-1}g P_r)_k^j D_H(P_r^{-1}g' P_t)_i^k$$

$$= / g P_r = P_s h \& g' P_t = P_r h' \Rightarrow gg' P_\epsilon = g P_r h' = P_s h h' \Leftrightarrow \delta_{st}(gg')$$

&  $\exists! P_r$  such that  $g P_r \in P_s H \Rightarrow$  sum over  $r$  gives just single nonzero contrib. ✓

$$= \delta_{st}(gg') D_H(P_s^{-1}gg' P_\epsilon)_i^j \quad \square$$

Theorem:  $D_H$  unitary  $\Rightarrow D_{G \oplus H}$  unitary

$$\underline{\text{Proof:}} \quad [D_G(g)^{-1}]_{ti}^{sj} = [D_G(g^{-1})]_{ti}^{sj} = \delta_{st}(g^{-1}) D_H(P_s^{-1}g^{-1}P_\epsilon)_i^j$$

$$= / g' P_\epsilon = P_s h \Leftrightarrow g P_r = P_\epsilon h' \Rightarrow \delta_{st}(g^{-1}) = \delta_{ts}(g) /$$

$$= \delta_{ts}(g) D_H((P_\epsilon^{-1}g P_s)^{-1})_i^j = \text{unitarity} / = \delta_{ts}(g) [D_H(P_\epsilon^{-1}g P_s)_j^i]^*$$

$$= [D_G(g)^+]_{ti}^{sj} \quad \square$$

• character of an induced degree

$$\chi_G(g) = \sum_s \delta_{ss}(g) D_H(p_s^{-1} g p_s)^j = \sum_s \delta_{ss}(g) \underset{\substack{\uparrow \\ H}}{X_H}(p_s^{-1} g p_s)$$

- summation over  $M$  selected elements  $p_s$  can be replaced by a sum over  $\#G/H$  with additional condition  $g'^{-1}gg' \in H \Rightarrow$  instead of a single representative of each coset we take every element from the coset; i.e.,  $\#H$  equal contributions instead of 1:

$$g p_s \in p_s H (\delta_{ss}(g)) \text{ & } g' \in p_s H \Rightarrow g'^{-1} g g' = (p_s h')^{-1} g (p_s h) \\ = h'^{-1} p_s^{-1} g p_s h' = h'^{-1} h h' \in H \Rightarrow gg' \in g' H = p_s H$$

$$\rightarrow \boxed{\chi_G(g) = \sum_s \delta_{ss}(g) X_H(p_s^{-1} g p_s) = \frac{1}{\#H} \sum_{\substack{g' \\ g'^{-1}gg' \in H}} X_H(g'^{-1} g g')}$$

- both expressions useful - in different situations

• decomposition of  $D_{H \times G} = D_G$

- assume we are inducing IRREP of  $H$ :  $\rho_G^{V \oplus G}$  is a degree of  $G$  induced from the  $\rho_H^V$  IRREP of  $H$ :

$$\rho_G^{V \oplus G} = \bigoplus_{\mu} \chi_{\mu}^{V \oplus G} \rho_{\mu}^G$$

$$\rho_H^{U \oplus H} = \bigoplus_{\nu} \chi_{\nu}^{U \oplus H} \rho_{\nu}^H$$

Theorem XXV: (Frobenius)

$$\boxed{\chi_{\mu}^{V \oplus G} = \chi_{\nu}^{U \oplus H}}$$

in words: IRREP  $S_G^{\alpha}$  of  $G$  is contained in  $S_G^{v \uparrow G}$  (60)  
as many times as is the IRREP  $S_H^v$  contained  
in  $S_H^{\alpha \downarrow H}$ ,  $\hookleftarrow$  very easy to determine!

$$\hookrightarrow \chi_G^{v \uparrow G}(g) = \sum_{\alpha} \alpha_v^{v \uparrow G} \chi_G^{\alpha}(g) = \sum_{\alpha} \alpha_v^{\alpha \downarrow H} \chi_G^{\alpha}(g)$$

Proof:  $\alpha_v^{v \uparrow G} = \frac{1}{\#G} \sum_g \chi_G^{\alpha}(g)^* \frac{1}{\#H} \sum_{\substack{g' \in G \\ g' \in gg' \in H}} \chi_H^v(g'^{-1}gg') =$

$\left/ \begin{array}{l} h = g'^{-1}gg' \Rightarrow g = g'hg'^{-1} \\ \Rightarrow \sum \sum = \sum \sum \end{array} \right/ = \frac{1}{\#G \#H} \sum_{h \in H} \chi_H^v(h) \underbrace{\sum_{g'} \chi_G^{\alpha}(g'hg'^{-1})^*}_{\#G \times \text{the same!}}$

$= \frac{1}{\#H} \sum_{h \in H} \chi_H^v(h) \chi_G^{\alpha}(h)^* = (\alpha_v^{\alpha \downarrow H})^* = \alpha_v^{\alpha \downarrow H}$   $\square$

Example: 1,  $H = \{e\}$ ,  $D_H$  is trivial hence  $\Rightarrow D_{H \uparrow G}$  is regular repre

# SYMMETRIES IN QM

52

- $G$  is a symmetry group of a system  
 $\Leftrightarrow \hat{H}$  (Schr. eq.) invariant with resp. to symmetry operations from  $G$
- what does it mean?
- how is the theory of use? useful?
- description of q. system - vector from Hilbert space  $\mathcal{H}$   
 $\rightarrow 1$  spinless particle  $\Rightarrow \psi \in C^2(\mathbb{R}^3)$  (bound states)
- action of  $G$  on  $\mathcal{H} \Rightarrow$  typically  $d$ -dim unitary representation
- $\rho: G \rightarrow \text{ISO}(\mathcal{H})$
- non-relativistic QM:  $G$  typically  $O(3), SO(3)$ , point groups, crystallographic groups

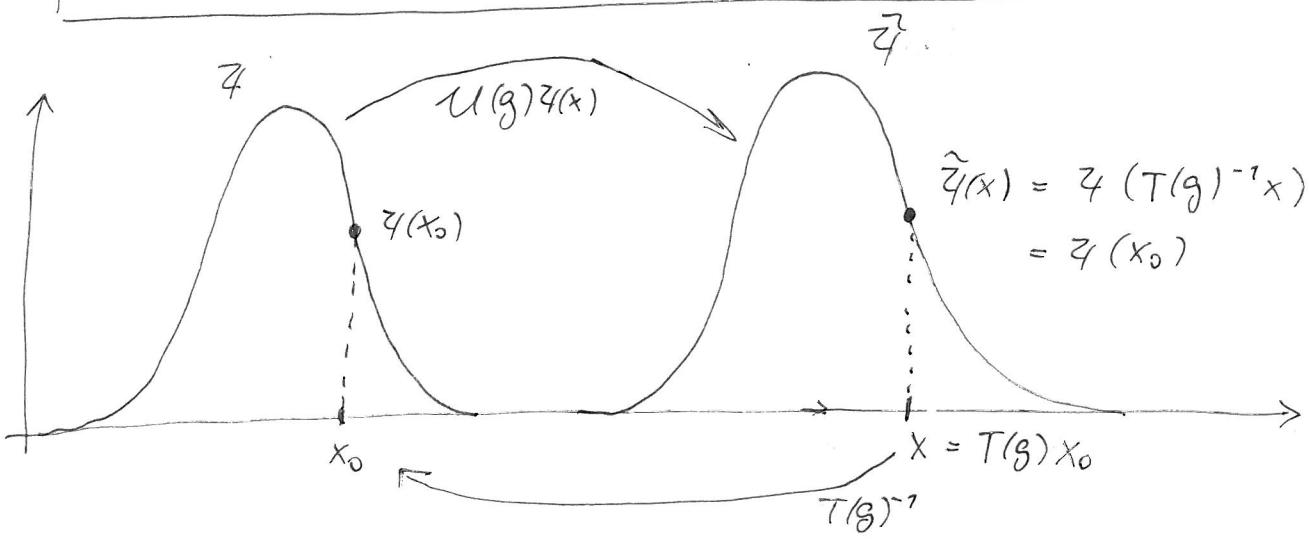
## Action of $G$ on $C^2(\mathbb{R}^3)$

1, action of  $G$  on  $\mathbb{R}^3: g \mapsto T(g) \in \text{Aut}(\mathbb{R}^3)$

$$\boxed{T(g)x} \quad \dots \text{coordinate transformation}$$

2, corresp. unitary op.  $U(g) \in \text{ISO}(C^2(\mathbb{R}^3)):$

$$\boxed{\tilde{\psi}(x) = U(g)\psi(x) = \psi(T(g)^{-1}x) \quad \forall \psi \in C^2(\mathbb{R}^3)}$$



•  $U(g)$  is indeed a representation of  $G$ :

$$U(g_1)U(g_2)\psi(x) = U(g_1)\psi(T(g_2)^{-1}x) = \psi(T(g_2)^{-1}T(g_1)^{-1}x)$$

↑  
note the order,  $T(g_1)$  acts directly  
on  $x$

$$= \psi([T(g_1)T(g_2)]^{-1}x) = \psi(T(g_1g_2)^{-1}x) = U(g_1g_2)\psi(x) \quad \square$$

### Transformation of operators

•  $\psi \mapsto U(g)\psi \Rightarrow A \mapsto \hat{A}$  such that matrix elements remain unchanged

→ This must hold for any  $U(g)$  generated by coordinate transformation, regardless symmetry - shifting/rotating whole system in space can't change physics

$$\Rightarrow \langle \psi | A | \psi \rangle = \langle U(g)\psi | \hat{A} | U(g)\psi \rangle$$

|| unitarity

$$\langle \psi | U(g)^+ \hat{A} U(g) | \psi \rangle$$

$$\Rightarrow \boxed{\hat{A} = U(g) A U(g)^+}$$

• what does it mean in "x-representation":

$$\phi(x) = A(x)\psi(x) \xrightarrow{U(g)} \phi(T(g)^{-1}x) = A(T(g)^{-1}x)\psi(T(g)^{-1}x)$$

$$U(g) A(x) \psi(x) = A(T(g)^{-1}x) U(g) \psi(x)$$

$$= \hat{A}(x) U(g) \psi(x)$$

$$\Rightarrow \boxed{\hat{A}(x) = U(g) A U(g)^+ = A(T(g)^{-1}x)}$$

Note: • multi-component  $\psi$  (bispinors, ...) ... individual components might mix under action of  $G \Rightarrow$

$$U(g) \begin{pmatrix} \psi_1(x) \\ \vdots \\ \psi_n(x) \end{pmatrix} = D(g) \begin{pmatrix} \psi_1(T(g)^{-1}x) \\ \vdots \\ \psi_n(T(g)^{-1}x) \end{pmatrix} \quad \text{with } D(g) \text{ some } 4\text{-dim. degree of } G$$

## Hamiltonian transformation

$$H \xrightarrow{g} U(g) H U(g)^*$$

- $g \in G$  symmetry group of a system ( $\Leftrightarrow H$  invariant)

$$\Rightarrow H U(g) = U(g) H \quad \forall g \in G$$

Note: •  $U(g)$  is not from IRREP  $\Rightarrow$  does not imply  $H = \lambda \mathbb{1}$   
 but ...

## eigenfunctions

$$H\psi = \lambda\psi \xrightarrow{g} U(g)H\psi \stackrel{[H, U] = 0}{=} HU(g)\psi = \lambda U(g)\psi$$

$\Rightarrow$  subspace  $\mathcal{H}_\lambda \subset \mathcal{H}$  of eigenfunctions corresp. to (possibly degenerate)  $\lambda$  is invariant under action of  $G$

$\Rightarrow$  basis of  $\mathcal{H}_\lambda$  forms basis of a rep of  $G$  on  $\mathcal{H}_\lambda$ :

$$U(g)\psi_{\lambda,n} = \sum_m \psi_{\lambda,m} D^\lambda(g)_m^{\mu} \quad \text{span}(\{\psi_{\lambda,1}, \dots, \psi_{\lambda,d}\}) = \mathcal{H}_\lambda$$

1,  $\mathcal{H}_\lambda$  does not contain proper invar. subspace

$\Rightarrow D^\lambda$  is IRREP & its dimension corresponds

to the degree of degeneracy of  $\lambda$

(note that indeed  $H = \lambda \mathbb{1}$  on  $\mathcal{H}^\lambda$  as required by Schur)

$\Rightarrow$  symmetry explains degeneracy of an energy level:

- if the eigenfunc. transforms as multi-dim IRREP then the level must be degenerate

- ground state typically totally sym  $\leftrightarrow$  trivial IRREP  
 $\Rightarrow$  non-degenerate

$\Rightarrow$  this is normal/geometrical degeneracy

2,  $\mathcal{H}_A$  reducible

a) accidental degeneracy

- due to specific values of some constants  
(ie, for specific geometry)

b) hidden (usually dynamical) symmetry

- true sym. group is larger  $\Rightarrow$  higher-dim. IRREP

Examples: 1) hidden symmetry - H atom

. apparent sym. group is  $SO(3) \Rightarrow E_{\text{ul}} = E_{\text{u}}$  seems accidental

. additional symmetry - Laplace-Runge-Lenz vector

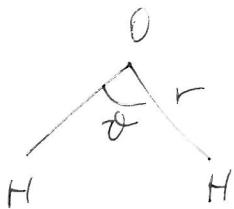
(remember Kepler problem:  $\vec{A} = \vec{p} \times \vec{r} - mkr^2 \hat{r}$ )

$$A_{ij} = -mkr^2 \hat{q}_j + \frac{1}{2} \sum k q_{ij} (p_i l_j + l_j p_i) \quad \leftarrow [l_i, p_j] \neq 0$$

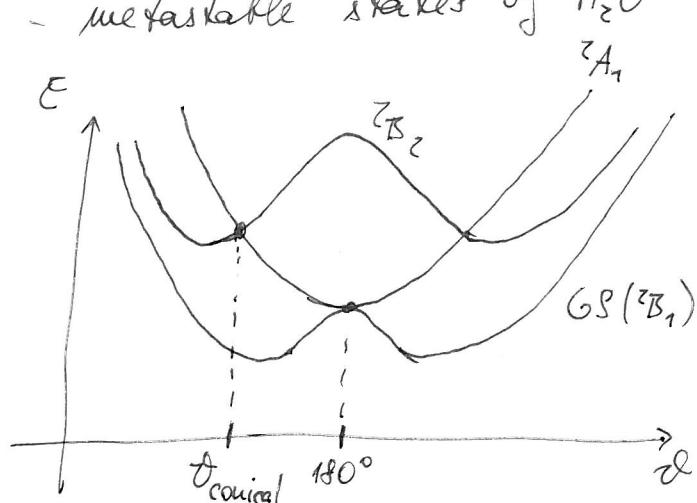
$\Rightarrow$  full sym. group is  $SO(4)/\mathbb{Z}_2 \sim SO(3) \otimes SO(3)$

$\Rightarrow$  explains the degeneracy

2) accidental degeneracy - metastable states of  $H_2O^-$



$C_{2v}$	$E$	$C_2$	$\sigma_v$	$\sigma_v'$
$A_1$	1	1	1	1
$A_2$	1	1	-1	-1
$B_1$	1	-1	1	-1
$B_2$	1	-1	-1	1



$\cdot \theta_{\text{conical}} \dots$  true accidental degeneracy ( $G$  is  $C_{2v}$ )

$\cdot \theta = 180^\circ \dots$  sym. group is  $D_{\text{oh}}$  & GS is of  $\Gamma_{\text{u}}$  sym.

$C_{2v} \leftrightarrow D_{\text{oh}}$ :

	$E \leftrightarrow E$	$C_2 \leftrightarrow \infty C_2$	$\sigma_v \leftrightarrow \sigma_v$	$\sigma_v' \leftrightarrow \infty \sigma_v'$	
$\Gamma_{\text{u}}$	2	0	2	0	$= A_1 \oplus B_2$

NOTE: here we consider  $C_{2v} \subset D_{\text{oh}}$  & this is subduction!

This document is provided by the **Chemical Portal** www.webqc.org

## D<sub>∞h</sub> point group

**not Abelian, ∞ irreducible representations**

**Character table**

	E	$2C_{\infty}^{\varphi}$	...	$\infty\sigma_v$	i	$2S_{\infty}^{\varphi}$	...	$\infty C_2'$	linear functions, rotations	quadratic
<b>A<sub>1g</sub>=Σ<sup>+</sup><sub>g</sub></b>	1	1	...	1	1	1	...	1		$x^2+y^2, z^2$
<b>A<sub>2g</sub>=Σ<sup>-</sup><sub>g</sub></b>	1	1	...	-1	1	1	...	-1	R <sub>z</sub>	
<b>E<sub>1g</sub>=Π<sub>g</sub></b>	2	2cos(φ)	...	0	2	-2cos(φ)	...	0	(R <sub>x</sub> , R <sub>y</sub> )	(xz, yz)
<b>E<sub>2g</sub>=Δ<sub>g</sub></b>	2	2cos(2φ)	...	0	2	2cos(2φ)	...	0		(x <sup>2</sup> -y <sup>2</sup> , xy)
<b>E<sub>3g</sub>=Φ<sub>g</sub></b>	2	2cos(3φ)	...	0	2	-2cos(3φ)	...	0		
...	...	...	...	...	...	...	...	...		
<b>A<sub>1u</sub>=Σ<sup>+</sup><sub>u</sub></b>	1	1	...	1	-1	-1	...	-1	z	
<b>A<sub>2u</sub>=Σ<sup>-</sup><sub>u</sub></b>	1	1	...	-1	-1	-1	...	1		
<b>E<sub>1u</sub>=Π<sub>u</sub></b>	2	2cos(φ)	...	0	-2	2cos(φ)	...	0	(x, y)	
<b>E<sub>2u</sub>=Δ<sub>u</sub></b>	2	2cos(2φ)	...	0	-2	-2cos(2φ)	...	0		
<b>E<sub>3u</sub>=Φ<sub>u</sub></b>	2	2cos(3φ)	...	0	-2	2cos(3φ)	...	0		
...	...	...	...	...	...	...	...	...		

You may print and redistribute verbatim copies of this document.