Direct product representations

Def: Basis of a representation

Let (ρ, V) be a d-dim repre and $\{\psi_j\}_{j=1}^{d}$ is a basis of V such that

$$T(g)\,\psi_j = \sum_{i=1}^{d} \psi_i\, D(g)^i_j$$

Then $\{\psi_j\}$ is called basis of a representation.
It is said that ψ_j transforms as j-th column of ρ.

Theorem XXIV

Let $\{\psi_j^a\}$ forms a basis of d_a-dim repre (ρ^a, V^a) and $\{\varphi_l^b\}$ basis of a d_b-dim repre (ρ^b, V^b).
Then $\{\psi_j^a \varphi_l^b\}_{j=1,\dots,d_a}^{l=1,\dots,d_b}$ forms a basis of a direct product representation

$$\rho^{(a\times b)} \equiv \rho^a \otimes \rho^b$$

which satisfies

$$T(g)\,\psi_j^a \varphi_l^b = \sum_{ik} \psi_i^a \varphi_k^b\, D^a(g)^i_j\, D^b(g)^k_l = \sum_{ik} \psi_i^a \varphi_k^b\, D^{(a\times b)}(g)^{ik}_{jl}$$

- the matrix $D^{(a\times b)}(g)^{ik}_{jl}$ is direct product of matrices

$$D^{(a\times b)}(g) = D^{(a)}(g) \otimes D^{(b)}(g) = \left(\begin{array}{c|c} D^a(g)^1_1\, D^b(g) & D^a(g)^1_2\, D^b(g) \;\cdots \\ \hline D^a(g)^2_1\, D^b(g) & \ddots \\ \vdots & \end{array}\right)$$

- $\dim \rho^{(a\times b)} = d_a \cdot d_b$
- the basis of $\rho^{(a\times b)}$ is ordered $\{\psi_1^a \varphi_1^b, \psi_1^a \varphi_2^b, \dots, \psi_{d_a}^a \varphi_{d_b}^b\}$
- $D^{(a\times b)}$ is a repre: $(A\otimes B)(A'\otimes B') = AA' \otimes BB'$
  $\Rightarrow D^{(a\times b)}(g_1 g_2) = D^{(a\times b)}(g_1)\cdot D^{(a\times b)}(g_2)$ $\Big\}$ (Ex.)
- even if ρ^a & ρ^b are IRREPs, $\rho^{(a\times b)}$ is in general reducible

- character of a direct-product representation

$$\chi^{a\times b}(g) = \sum_{ik} D^{(a\times b)}(g)^{ik}_{ik} = \sum_{ik} D^a(g)^i_i \, D^b(g)^k_k = \chi^a(g)\chi^b(g)$$

$$\Rightarrow \boxed{\mu_\alpha^{a\times b} = \frac{1}{\#G}\sum_g \chi^\alpha(g)^* \chi^a(g)\chi^b(g)}$$ decomposition of a direct product representation

Example : • He atom (without spin)

$$\hat{H} = -\frac{1}{2}\Delta_1 - \frac{1}{r_1} - \frac{1}{2}\Delta_2 - \frac{1}{r_2} + \frac{1}{|r_1 - r_2|} = H_1 + H_2 + V_{int}$$

a) e^- non-interacting ($H_0 = H_1 + H_2$)

$\Rightarrow$ eigenfunctions of H_0 are products of eigenf. of H_1 & H_2, which are defined by n, l, m and form bases of IRREP's of $SO(3)$

$\Rightarrow |\psi(r_1, r_2)\rangle = |n_1 l_1 m_1\rangle |n_2 l_2 m_2\rangle$ form basis of $(2l_1+1)(2l_2+1)$-dim IRREP of a group $SO(3)\otimes SO(3)$

b) e^- interact via $V_{int} = \frac{1}{|r_1 + r_2|}$

$\Rightarrow$ the symmetry group is $SO(3)$

$\Rightarrow |n_1 l_1 m_1\rangle |n_2 l_2 m_2\rangle$ form basis of a reducible direct-product representation of $SO(3)$

$\Rightarrow$ can be decomposed to IRREP's defined by the total orbital momentum L

- decomposition of direct products of vector representations (useful for character tables)

- Wigner-Eckart theorem

- special case: symmetric & anti-symmetric products of two equivalent representations

- ψ_j, φ_ℓ ... two different bases of the equivalent representations

(- for instance, consider high-dimensional reducible representation containing two copies of the repre of interest $\Rightarrow$ ψ_j, φ_ℓ are bases of the two respective invariant subspaces)

$$\left.\begin{aligned} T(g)(\psi_j \varphi_\ell) &= \sum_{ik} (\psi_i \varphi_k) D(g)^i_j D(g)^k_\ell \\ T(g)(\psi_\ell \varphi_j) &= \sum_{ik} (\psi_i \varphi_k) D(g)^i_\ell D(g)^k_j \end{aligned}\right\} +, -$$

(+) $\Rightarrow T(g)(\psi_j \varphi_\ell + \psi_\ell \varphi_j) = \sum_{ik} (\psi_i \varphi_k) [D(g)^i_j D(g)^k_\ell + D(g)^i_\ell D(g)^k_j]$

$= /[\;]$ sym in $(i \leftrightarrow k)/ = \frac{1}{2} \sum_{ik} (\psi_i \varphi_k + \psi_k \varphi_i)(D^i_j D^k_\ell + D^i_\ell D^k_j)$

(−) $\Rightarrow T(g)(\psi_j \varphi_\ell - \psi_\ell \varphi_j) = \frac{1}{2} \sum_{ik} (\psi_i \varphi_k - \psi_k \varphi_i)(D^i_j D^k_\ell - D^i_\ell D^k_j)$

$\Rightarrow$ symmetric & anti-symmetric products of basis vectors generate invariant subspaces

$\Rightarrow \rho \otimes \rho = \{\rho \otimes \rho\} \oplus [\rho \otimes \rho]$

- $\dim \{\} = \#\{j, \ell \mid j \leq \ell\} = \frac{1}{2} d(d+1)$
- $\dim [\,] = \#\{j, \ell \mid j < \ell\} = \frac{1}{2} d(d-1)$
- characters (ex.): $\chi^{\{\}}(g) = \frac{1}{2}(\chi(g)^2 + \chi(g^2))$

  $\chi^{[\,]}(g) = \frac{1}{2}(\chi(g)^2 - \chi(g^2))$

Example: $\cdot\, \rho$ is vector repre $O(3)$ $\Rightarrow d = 3$

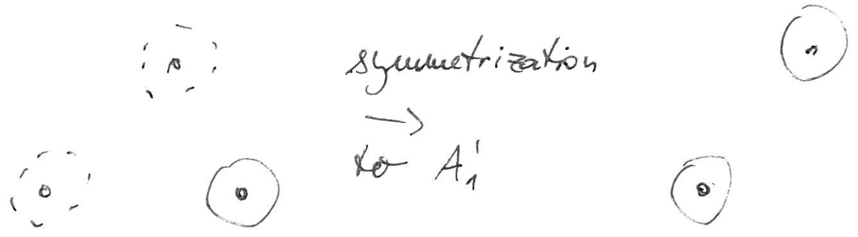
$\Rightarrow \underbrace{\{\rho \otimes \rho\} = \rho^s \oplus \rho^d}_{\text{quadratic functions}}$; $[\rho \otimes \rho]$ = pseudo-vec. repre (vec. for $SO(3)$)

quadratic functions ($s \Leftrightarrow x^2+y^2+z^2 \Leftrightarrow$ trivial repre)

PROJECTION (SYMMETRIZATION) OPERATORS

- way to find basis of an invariant subspace corresponding to specific repre (usually IRREP)
- also: given a set of vectors/functions, construct their linear combination that transform as a specific IRREP (symmetry adaptation)

Example: • 1s functions on H_3^{2+}



- derivation:
  - assume we know one basis vector ψ_i^μ & explicit form of the matrices $D^\mu(g)$ of an IRREP ρ^μ
    ⇒ it is possible to generate the rest of the basis:

$$T(g)\psi_i^\mu = \sum_j \psi_j^\mu D^\mu(g)^j_i \qquad / [(D^\mu(g))^r_s]^* \;,\; \sum_g$$

$$\sum_g [D^\mu(g)^r_s]^* T(g)\psi_i^\mu = \sum_j \psi_j^\mu \frac{\#G}{d_\mu}\delta_{rj}\delta_{si} = \frac{\#G}{d_\mu}\delta_{si}\psi_r^\mu$$

$$\Rightarrow /s=i/ \Rightarrow \quad \psi_r^\mu = \frac{d_\mu}{\#G}\sum_g [D^\mu(g)^r_i]^* T(g)\psi_i^\mu$$

⇒ from ψ_i^μ we can generate all the remaining „partner basis vectors" with resp. to ρ^μ

Def: Symmetrization operator

$$P_{rs}^\mu = \frac{d_\mu}{\#G}\sum_g [D^\mu(g)^r_s]^* T(g) \quad \Rightarrow \quad P_{rs}^\mu \psi_i^\mu = \psi_r^\mu \delta_{is} \qquad (+)$$

• P^{μ}_{rs} are called projection ops but are not projectors!

$$0 \overset{(+)}{=} P^{\mu}_{12} \psi^{\mu}_{1} = P^{\mu}_{12}\left(P^{\mu}_{12}\psi^{\mu}_{2}\right) \Rightarrow \left(P^{\mu}_{rs}\right)^2 \neq P^{\mu}_{rs}$$

• only "diagonal" P^{μ}_{ii} ops are self-adjoint projectors

$\Rightarrow$ algorithm: - basis of an invar. subspace corr. to IRREP D^{μ}

1, take $\psi \in W^{\mu} \subset V$ arbitrary, choose $1 \leq s \leq d_{\mu}$ fixed

2, generate d_{μ} vectors

$$\psi^{\mu}_{rs} = P^{\mu}_{rs}\psi \quad , r = 1, \dots, d_{\mu}$$

$\Rightarrow \{\psi^{\mu}_{rs}\}_r$ forms the desired basis, ψ^{μ}_{rs} transforms as r-th column:

$$T(h)\psi^{\mu}_{rs} = \sum_j \psi^{\mu}_{js} D^{\mu}(h)_r^{\ j}$$

Proof:

$$T(h)\psi^{\mu}_{rs} = \frac{d_{\mu}}{\#G}\sum_g \left[D^{\mu}(g)_s^{\ r}\right]^* T(hg)\psi = /hg = g' \Rightarrow g = h^{-1}g'/ =$$

$$= \frac{d_{\mu}}{\#G}\sum_{g'}\left[D^{\mu}(h^{-1}g')_s^{\ r}\right]^* T(g')\psi = \frac{d_{\mu}}{\#G}\sum_{g'}\sum_j \left[D^{\mu}(h^{-1})_j^{\ r} D^{\mu}(g')_s^{\ j}\right]^* T(g')\psi$$

$$= \sum_j \psi^{\mu}_{js} D^{\mu}(h)_r^{\ j} \quad \boxtimes$$

Note: • ψ need not to be from W^{μ} but must have nonzero projection onto W^{μ}

• the need for explicit matrix repre makes the approach impractical

$\Rightarrow$

Def: Incomplete symmetrization operator

$$P^{\mu} \equiv \sum_i P^{\mu}_{ii} = \frac{d_{\mu}}{\#G}\sum_g \chi^{\mu}(g)^* T(g)$$

- algorithm #2:
  - $\psi \in V$ arbitrary
    $$\Rightarrow P^{\mu}\psi = \sum_j \psi_{ij}^{\mu} \in W^{\mu}$$

1, take d_μ different vectors ψ_i from V

2, construct d_μ projections $\psi_i^{\mu} = P^{\mu}\psi_i$

3, orthogonalization

4,* if less than d_μ OG vectors remained after 3, then generate more ψ_j^{μ} from additional ψ_j's until the basis set is complete

Examples: 1, quadratic functions & D_{3h}

2, MO-LCAO for H_3^+ - after QM intro

SYMMETRIES IN QM

- G is a symmetry group of a system
  $\Leftrightarrow$ $\hat{H}$ (Schr. eq.) invariant with resp. to symmetry operations from G

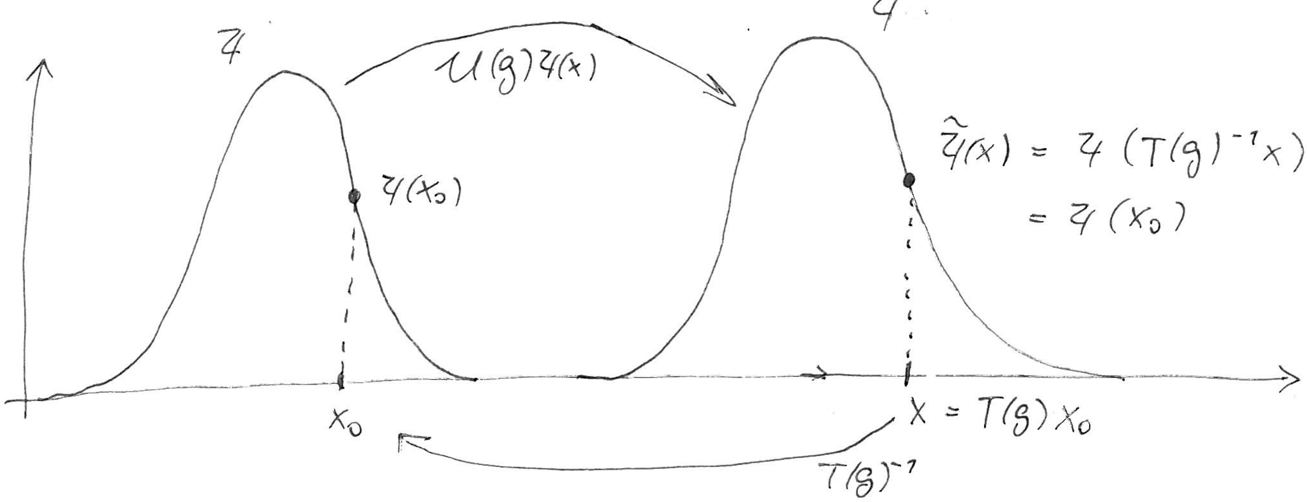
  → what does it mean?
  → how is the theory of repre useful?

- description of q. system – vector from Hilbert space $\mathcal{H}$
  → 1 spinless particle $\Rightarrow$ $\psi \in L^2(\mathbb{R}^3)$ (bound states)
- action of G on $\mathcal{H}$ $\Rightarrow$ typically ∞-dim unitary representation
  $$\rho : G \to \mathrm{ISO}(\mathcal{H})$$
- non-relativistic QM: G typically $O(3), SO(3)$, point groups, crystalographic groups

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

1/ action of G on $\mathbb{R}^3$: $g \mapsto T(g) \in \mathrm{Aut}(\mathbb{R}^3)$
$$\boxed{x' = T(g)x} \quad \text{... coordinate transformation}$$

2/ corresp. unitary op. $\mathcal{U}(g) \in \mathrm{ISO}(L^2(\mathbb{R}^3))$:
$$\boxed{\tilde{\psi}(x) = \mathcal{U}(g)\psi(x) \equiv \psi(T(g)^{-1}x) \quad \forall \psi \in L^2(\mathbb{R}^3)}$$



- $\mathcal{U}(g)$ is indeed a representation of G:

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

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

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

Transformation of operators

- $\psi \mapsto \mathcal{U}(g)\psi \Rightarrow A \mapsto \hat{A}$ such that matrix elements remain unchanged
  - → this must hold for any $\mathcal{U}(g)$ generated by coordinate transformation, regardless symmetry - shifting/rotating whole system in space can't change physics

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

|| unitarity

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

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

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

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

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

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

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

Note: • multi-component ψ (bispinors, ...) ... individual components might mix under action of G ⇒

$$\mathcal{U}(g)\begin{pmatrix}\psi_1(x)\\ \vdots \\ \psi_4(x)\end{pmatrix} = D(g)\begin{pmatrix}\psi_1(T(g)^{-1}x)\\ \vdots \\ \psi_4(T(g)^{-1}x)\end{pmatrix}$$

with $D(g)$ some 4-dim. repre of G

- Hamiltonian transformation

$$H \overset{g}{\longmapsto} \mathcal{U}(g)\, H\, \mathcal{U}(g)^{+}$$

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

$$\Rightarrow \quad H\,\mathcal{U}(g) = \mathcal{U}(g)\,H \qquad \forall g \in G$$

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

but ...

- eigenfunctions

$$H\psi = \lambda\psi \overset{g}{\longmapsto} \mathcal{U}(g) H \psi \overset{[H,\mathcal{U}]=0}{=} H\,\mathcal{U}(g)\psi = \lambda\,\mathcal{U}(g)\psi$$

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

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

$$\mathcal{U}(g)\,\psi_{\lambda,n} = \sum_m \psi_{\lambda,m}\, D^\lambda(g)^m{}_n \qquad \mathrm{span}\left(\{\psi_{\lambda,1}, \dots, \psi_{\lambda,d}\}\right) = \mathcal{H}_\lambda$$

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

$\Rightarrow$ D^λ is IRREP & it's dimension corresponds to the degree of degeneracy of λ

(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, $\mathcal{H}_\lambda$ reducible

a) <u>accidental degeneracy</u>

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

b) <u>hidden</u> (usually dynamical) <u>symmetry</u>

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

<u>Examples:</u> 1, <u>hidden symmetry</u> – H atom

- apparent sym. group is $SO(3)$ $\Rightarrow$ $E_{nl} = E_n$ seems accidental
- additional symmetry – Laplace-Runge-Lenz vector

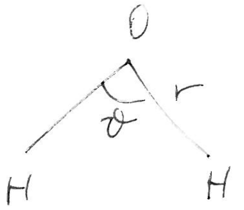
(remember Kepler problem: $\vec{A} = \vec{p} \times \vec{L} - mk\hat{\vec{r}}$)

$$A_q = -mk\hat{r}_q + \frac{1}{2}\varepsilon_{qij}(p_i l_j + l_j p_i) \quad \Leftarrow [l_i, p_j] \neq 0$$

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

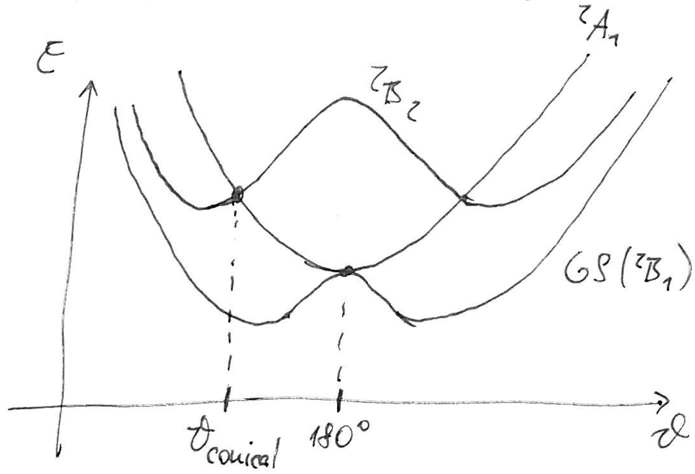
$\Rightarrow$ explains the degeneracy

2, <u>accidental degeneracy</u> – metastable states of H_2O^-



$\Rightarrow$

C_{2v}	E	C_2	σ_v	σ_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



- $\vartheta_{conical}$ ... true accidental degeneracy (G is C_{2v})
- $\vartheta = 180°$ ... sym. group is $D_{\infty h}$ & GS is of Π_u sym.

$C_{2v} \leftrightarrow D_{\infty h}$:

	$E \leftrightarrow E$	$C_2 \leftrightarrow \infty C_2$	$\sigma_v \leftrightarrow S_1$	$\sigma_v' \leftrightarrow \infty\sigma_v$	
Π_u	2	0	2	0	$= A_1 \oplus B_2$

<u>NOTE:</u> • here we consider $C_{2v} < D_{\infty h}$ & this is subduction!

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$D_{\infty h}$ 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**
$A_{1g}=\Sigma^+_g$	1	1	...	1	1	1	...	1		x^2+y^2, z^2
$A_{2g}=\Sigma^-_g$	1	1	...	-1	1	1	...	-1	R_z	
$E_{1g}=\Pi_g$	2	2cos(φ)	...	0	2	-2cos(φ)	...	0	(R_x, R_y)	(xz, yz)
$E_{2g}=\Delta_g$	2	2cos(2φ)	...	0	2	2cos(2φ)	...	0		(x^2-y^2, xy)
$E_{3g}=\Phi_g$	2	2cos(3φ)	...	0	2	-2cos(3φ)	...	0		
...	...	...	...	...	...	...	...	...		
$A_{1u}=\Sigma^+_u$	1	1	...	1	-1	-1	...	-1	z	
$A_{2u}=\Sigma^-_u$	1	1	...	-1	-1	-1	...	1		
$E_{1u}=\Pi_u$	2	2cos(φ)	...	0	-2	2cos(φ)	...	0	(x, y)	
$E_{2u}=\Delta_u$	2	2cos(2φ)	...	0	-2	-2cos(2φ)	...	0		
$E_{3u}=\Phi_u$	2	2cos(3φ)	...	0	-2	2cos(3φ)	...	0		
...	...	...	...	...	...	...	...	...		