# Direct product representations

Def: Basis of a representation

Let $(\rho, V)$ 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 <u>basis of a representation</u>.

It is said that <u>$\psi_j$ transforms as $j$-th column</u> of $\rho$.

<u>Theorem XXIV</u>

Let $\{\psi_j^a\}$ forms a basis of $d_a$-dim repre $(\rho^a, V^a)$ and $\{\varphi_\ell^b\}$ basis of a $d_b$-dim repre $(\rho^b, V^b)$.

Then $\{\psi_j^a \varphi_\ell^b\}_{j=1,\dots,d_a}^{\ell=1,\dots,d_b}$ forms a basis of a <u>direct product representation</u>

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

which satisfies

$$T(g)\psi_j^a \varphi_\ell^b = \sum_{ik} \psi_i^a \varphi_k^b D^a(g)^i_j D^b(g)^k_\ell = \sum_{ik} \psi_i^a \varphi_k^b D^{(a\times b)}(g)^{ik}_{j\ell}$$

- the matrix $D^{(a\times b)}(g)^{ik}_{j\ell}$ 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: $(A\otimes B)(A'\otimes B') = AA' \otimes BB'$
  $\Rightarrow D^{(a\times b)}(g_1 g_2) = D^{(a\times b)}(g_1)\cdot D^{(a\times b)}(g_2)$ } (Ex.)
- even if $\rho^a$ & $\rho^b$ 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

- $\psi_j, \varphi_l$ ... two different bases of the equivalent representations

(– for instance, consider high-dimensional reducible representation containing two copies of the repre of interest ⇒ $\psi_j, \varphi_l$ are bases of the two respective invariant subspaces)

$$\left.\begin{aligned} T(g)(\psi_j\varphi_l) &= \sum_{ik}(\psi_i\varphi_k)\,D(g)^i_j\,D(g)^k_l \\ T(g)(\psi_l\varphi_j) &= \sum_{ik}(\psi_i\varphi_k)\,D(g)^i_l\,D(g)^k_j \end{aligned}\right\} +,-$$

(+) $\Rightarrow T(g)(\psi_j\varphi_l+\psi_l\varphi_j) = \sum_{ik}(\psi_i\varphi_k)\left[D(g)^i_jD(g)^k_l + D(g)^i_lD(g)^k_j\right]$

$= /[\;]\text{ sym in }(i\leftrightarrow k)/ = \frac{1}{2}\sum_{ik}(\psi_i\varphi_k+\psi_k\varphi_i)(D^i_jD^k_l+D^i_lD^k_j)$

(−) $\Rightarrow T(g)(\psi_j\varphi_l-\psi_l\varphi_j) = \frac{1}{2}\sum_{ik}(\psi_i\varphi_k-\psi_k\varphi_i)(D^i_jD^k_l-D^i_lD^k_j)$

⇒ symmetric & anti-symmetric products of basis vectors generate invariant subspaces

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

- $\dim\{\} = \#\{j,l\,|\,j\le l\} = \frac{1}{2}d(d+1)$
- $\dim[\,] = \#\{j,l\,|\,j<l\} = \frac{1}{2}d(d-1)$
- characters (ex.): $\chi^{\{\}}(g) = \frac{1}{2}\left(\chi(g)^2+\chi(g^2)\right)$

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

Example: • $\rho$ is vector repre $O(3)$ ⇒ $d=3$

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

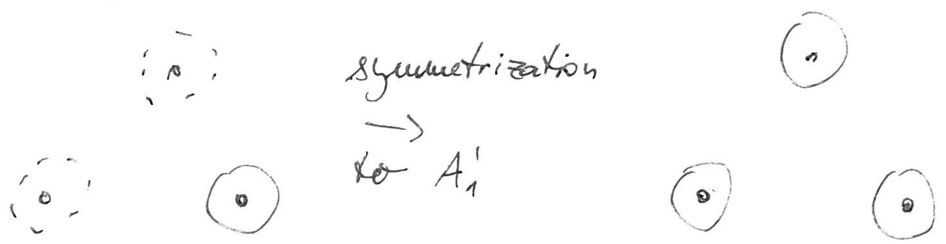
→ quadratic functions ($s \Leftrightarrow x^2+y^2+z^2 \Leftrightarrow$ trivial repre)

## 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 $\psi_i^{\mu}$ & explicit form of the matrices $D^{\mu}(g)$ of an IRREP $\rho^{\mu}$
    $\Rightarrow$ it is possible to generate the rest of the basis:

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

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

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

$\Rightarrow$ from $\psi_i^{\mu}$ we can generate all the remaining „partner basis vectors" with resp. to $\rho^{\mu}$

**Def:** Symmetrization operator

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

• $P^{\mu}_{rs}$ 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" $P^{\mu}_{ii}$ ops are self-adjoint projectors

⇒ algorithm: – basis of an invar. subspace corr. to IRREP $\mu$

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

2, generate $d_{\mu}$ vectors

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

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

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

Proof:

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

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

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

Note:
• $\psi$ need not to be from $W^{\mu}$ but must have nonzero projection onto $W^{\mu}$
• the need for explicit matrix repre makes the approach impractical

⇒

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 $d_\mu$ different vectors $\psi_i$ from $V$

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

3, orthogonalization

4,* if less than $d_\mu$ OG vectors remained after 3, then generate more $\psi_j^{\mu}$ from additional $\psi_j$'s until the basis set is complete

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

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