Group theory

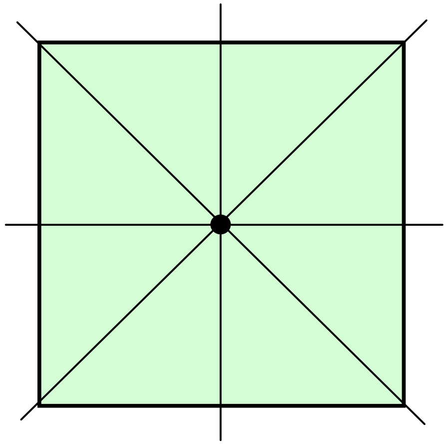
Definition: group $\mathcal{G}$ is a set $\mathcal{G} = \{a, b, c, \ldots\}$ with a product $\cdot$

$a \in \mathcal{G}$, $b \in \mathcal{G}$ $\Rightarrow$ $a \cdot b \in \mathcal{G}$ associative $(a \cdot b) \cdot c = a \cdot (b \cdot c)$

identity $E \in \mathcal{G}$ with $E \cdot a = a \cdot E = a$

inverse $a \in \mathcal{G} \Rightarrow a^{-1} \in \mathcal{G}$ with $a^{-1} \cdot a = a \cdot a^{-1} = E$

Example: C_{4v} symmetry operation of square



$$C_{4v} = \{E, C_4, C_4^{-1}, C_2, \sigma_h, \sigma_h', \sigma_d, \sigma_d'\}$$

$$C_4 \cdot C_4 = C_2 \qquad \underbrace{\sigma_h \cdot C_4 = \sigma_d' \qquad C_4 \cdot \sigma_h = \sigma_d}_{\sigma_h \cdot C_4 \neq C_4 \cdot \sigma_h}$$

non-abelian

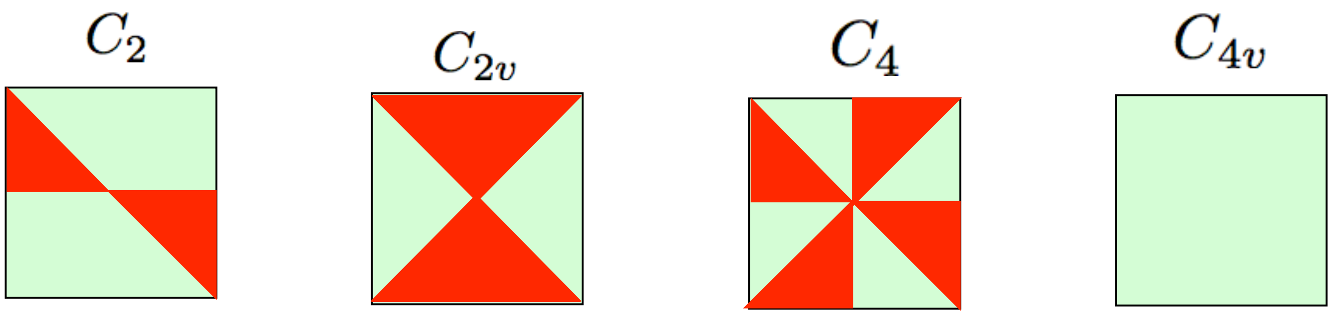
Group theory

subgroup: group $\mathcal{G}'$ subset of $\mathcal{G}$

$$\mathcal{G}' \subset \mathcal{G}$$

examples:

$$\left.\begin{aligned} C_4 &= \{E, C_4, C_4^{-1}, C_2\} \\ C_{2v} &= \{E, C_2, \sigma_h, \sigma_h'\} \\ C_2 &= \{E, C_2\} \end{aligned}\right\} \subset C_{4v}$$



number of elements: $|\mathcal{G}'|$ devides $|\mathcal{G}|$

Group representation

linear transformations: consider n-dimensional vector space $\mathcal{V} = \{|1\rangle, |2\rangle, \dots, |n\rangle\}$

transformations on $\mathcal{V}$ by unitary n x n-matrices $|k'\rangle = g|k\rangle = \sum_j M_{k'j}(g)|j\rangle$

matrices $\hat{M}$ satisfies all properties of a group

representation

mapping (homomorphism) of group $\mathcal{G}$ on n x n -matrices in $\mathcal{V}$

$g \quad \rightarrow \quad \hat{M}(g)$ conserving group structure ➡ representation of $\mathcal{G}$

$$\hat{M}(E) = \hat{1}_{n\times n} \qquad \hat{M}(g^{-1}) = \hat{M}(g)^{-1}$$

equivalent representations: $\hat{M}'(g) = \hat{U}\hat{M}(g)\hat{U}^{-1}$ basis transformation $\hat{U}$

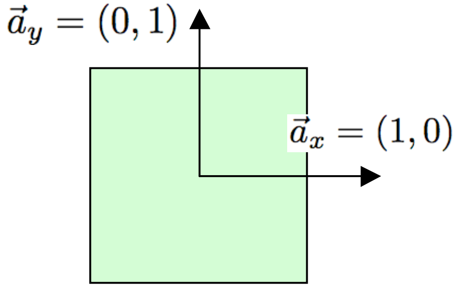
characters: $\chi(g) = tr\hat{M}(g)$ independent of basis

Group representation

irreducible representation: independent of basis $\{\hat{M}(g)\}$ connects whole $\mathcal{V}$

trivial representation: *n = 1* $g \to \hat{M}(g) = 1$

example: C_{4v} $\hat{M}$ transformation of $\{\vec{a}_x, \vec{a}_y\}$



$$E \to \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad C_4 \to \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \quad C_4^{-1} \to \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \quad C_2 \to \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\sigma_h \to \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad \sigma_h' \to \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \quad \sigma_d \to \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_d' \to \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}$$

character table

	E	C_4	C_4^{-1}	C_2	σ_h	σ_h'	σ_d	σ_d'	basis function
A_1	1	1	1	1	1	1	1	1	1
A_2	1	1	1	1	-1	-1	-1	-1	$xy(x^2-y^2)$
B_1	1	-1	-1	1	1	1	-1	-1	x^2-y^2
B_2	1	-1	-1	1	-1	-1	1	1	xy
E	2	0	0	-2	0	0	0	0	$\{x,y\}$

Group representation & quantum mechanics

symmetry operations of Hamiltonian form a group $\mathcal{G} = \{\hat{S}_1, \ldots\}$

Hilbertspace is vector space $\{|\psi_1\rangle, \ldots\}$

stationary states: $\mathcal{H}|\phi_n\rangle = \epsilon_n|\phi_n\rangle$

$$[\hat{S}, \mathcal{H}] = 0 \quad \Rightarrow \quad \mathcal{H}\hat{S}|\phi_n\rangle = \hat{S}\mathcal{H}|\phi_n\rangle = \epsilon_n \hat{S}|\phi_n\rangle$$

$|\phi_n\rangle$ and $|\phi'_n\rangle = \hat{S}|\phi_n\rangle$ degenerate

degenerate states form a vector space with an irred. representation of $\mathcal{G}$

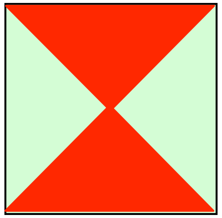
$$\{|\phi_1\rangle, \ldots, |\phi_m\rangle\} \quad \text{with} \quad \hat{S}|\phi_k\rangle = \sum_{k'=1}^{m} M_{kk'}|\phi_{k'}\rangle$$

dimension *m* of representation = degeneracy

Group representation & quantum mechanics

symmetry lowering $C_{4v} \rightarrow C_{2v}$

C_{2v}



	E	C_2	σ_h	σ_h'	basis
A_1'	1	1	1	1	1
A_2'	1	-1	1	-1	x
B_1'	1	1	-1	-1	xy
B_2'	1	-1	-1	1	y

C_{4v}	C_{2v}
A_1	A_1'
A_2	B_1'
B_1	A_1'
B_2	B_1'
E	$A_2' \oplus B_2'$

splitting of degeneracy through symmetry lowering