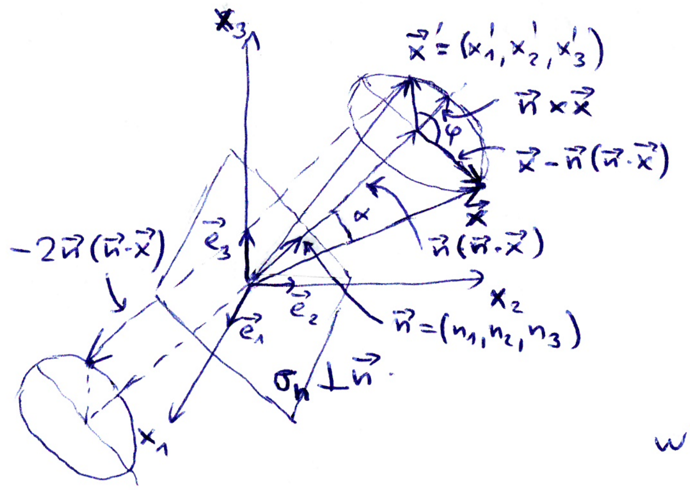
Tutorial: Vector and pseudovector representations

T3

1) Vector representation Γ^V – action of a point group on $\mathbb{R}^3$



– in general for a group G and a vector $\vec{x}$ we have

$$\vec{x} = \sum_{i=1}^{3} x_i \vec{e}_i \xrightarrow{g\in G} \vec{x}' = \sum_{i=1}^{3} x_i' \vec{e}_i$$

action of g on $\vec{x}$ where g is either rotation or improper rotation

where $x_i' = \sum_{k=1}^{3} \underbrace{D^V_{ij}(g)}_{} x_j$ form 3-dim. matrix vector representation of G

- from the figure, we can see that the resulting vector $\vec{x}'$ obtain from $\vec{x}$ by rotation around $\vec{n}$ by φ can be expressed as

$$\vec{x}' = \vec{n}(\vec{n}\cdot\vec{x}) + \cos\varphi\,[\vec{x} - \vec{n}(\vec{n}\cdot\vec{x})] + \sin\varphi\,(\vec{n}\times\vec{x})$$

(because $\vec{n}\times\vec{x}$ has the direction perpendicular to $\vec{n}$ and $\vec{x}$ and the magnitude $|\vec{n}\times\vec{x}| = |\vec{x}|\sin\alpha = |\vec{x} - \vec{n}(\vec{n}\cdot\vec{x})|$ where α is the angle between $\vec{n}$ and $\vec{x}$)

and thus

$$D^V_{ij}(C^{\vec{n}}_{\varphi}) = \delta_{ij}\cos\varphi + (1-\cos\varphi)n_i n_j + \sum_{k=1}^{3}\varepsilon_{ikj} n_k \sin\varphi$$

(note that $(\vec{n}\times\vec{x})_i = \sum_{j,k}\varepsilon_{ijk} n_j x_k$)

- if we subtract $2\vec{n}(\vec{n}\cdot\vec{x})$ from $\vec{x}'$ after rotation, we get an image of $\vec{x}$ after the improper rotation $S^{\vec{n}}_{\varphi}$

and $$D^V_{ij}(S^{\vec{n}}_{\varphi}) = \delta_{ij}\cos\varphi + (-1-\cos\varphi)n_i n_j + \sum_{k=1}^{3}\varepsilon_{ikj} n_k$$

only here we change the sign

- for characters of this representation, we have

$$\chi^V(C^{\vec{n}}_{\varphi}) = \mathrm{Tr}\, D^V(C^{\vec{n}}_{\varphi}) = 3\cos\varphi + (1-\cos\varphi)\sum_{i=1}^{3} n_i^2 = 1 + 2\cos\varphi$$

$$\chi^V(S^{\vec{n}}_{\varphi}) = \mathrm{Tr}\, D^V(S^{\vec{n}}_{\varphi}) = 3\cos\varphi + (-1-\cos\varphi)\cdot 1 = -1 + 2\cos\varphi$$

both independent of $\vec{n}$ (as all proper (or improper) rotations by the same angle φ in $O(3)$ form a conjugacy class)

- we can get the characters quickly from any rotation, for example from rotation around the axis z:

$$D^{V}(C_\varphi^{z}) = \begin{pmatrix} \cos\varphi & -\sin\varphi & 0 \\ \sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \text{giving} \quad \chi^{V}(C_\varphi) = 1 + 2\cos\varphi$$

and $$D^{V}(S_\varphi^{z}) = \begin{pmatrix} \cos\varphi & -\sin\varphi & 0 \\ \sin\varphi & \cos\varphi & 0 \\ 0 & 0 & -1 \end{pmatrix} \quad \text{giving} \quad \chi^{V}(S_\varphi) = -1 + 2\cos\varphi$$

- for the group $O(3)$ and its subgroups $SO(3), T, T_d, T_h, O, O_h, I,$ and I_h, (if we restrict the repr. only to elements of a particular group) the vector representation is irreducible, but for smaller point groups, it is reducible and we usually take as the main C_n axis the z-axis and we set the structure of the matrix $\begin{pmatrix} & & 0 \\ & & 0 \\ 0 & 0 & \boxed{\pm 1} \end{pmatrix}$
  - the subrepresentation in (x,y) can be for certain point groups further decomposed to one-dimens. repr.

2) <u>pseudovector representation Γ^{PV}</u>

- consider two vectors $\vec{x}$ and $\vec{y}$ transformed under $g \in G$ into vectors $\vec{x}\,'$ and $\vec{y}\,'$ with components

$$x_i' = \sum_{k=1}^{3} D^{V}_{ik}(g)\, x_k \quad \text{and} \quad y_j' = \sum_{\ell=1}^{3} D^{V}_{j\ell}(g)\, y_\ell$$

- how does $\vec{R} = \vec{x} \times \vec{y}$, i.e. $R_i = \sum_{j,k} \varepsilon_{ijk}\, x_j\, y_k$ transform?
- we get for example

$$R_1' = x_2' y_3' - x_3' y_2' = \sum_{k,\ell} D^{V}_{2k}(g)\, D^{V}_{3\ell}(g)\,(x_k y_\ell - x_\ell y_k) =$$

according to Cramer's rule $\rightarrow$
$$= \underbrace{(D^{V}_{22} D^{V}_{33} - D^{V}_{23} D^{V}_{32})}_{(\det D^{V})(D^{V-1})_{11}} R_1 + \underbrace{(D^{V}_{23} D^{V}_{31} - D^{V}_{21} D^{V}_{33})}_{(\det D^{V})(D^{V-1})_{21}} R_2 + \underbrace{(D^{V}_{21} D^{V}_{32} - D^{V}_{22} D^{V}_{31})}_{(\det D^{V})(D^{V-1})_{31}} R_3$$

orthogonality of $D^{V}(g)$ $\rightarrow$
$$= (\det D^{V})\,(D^{V}_{11} R_1 + D^{V}_{12} R_2 + D^{V}_{13} R_3)$$

and similarly for R_2' and R_3'

- thus $$\vec{R}\,' = [\det D^{V}(g)]\, D^{V}(g)\, \vec{R} = \underbrace{D^{PV}(g)}_{\text{pseudovector representation}}\, \vec{R}$$

with characters

$$\chi^{PV}(C_\varphi) = 1 + 2\cos\varphi \quad \text{and} \quad \chi^{PV}(S_\varphi) = 1 - 2\cos\varphi = -\chi^{V}(S_\varphi)$$

(the same as $\chi^{V}(C_\varphi)$) as $\det D^{V}(S_\varphi) = -1$