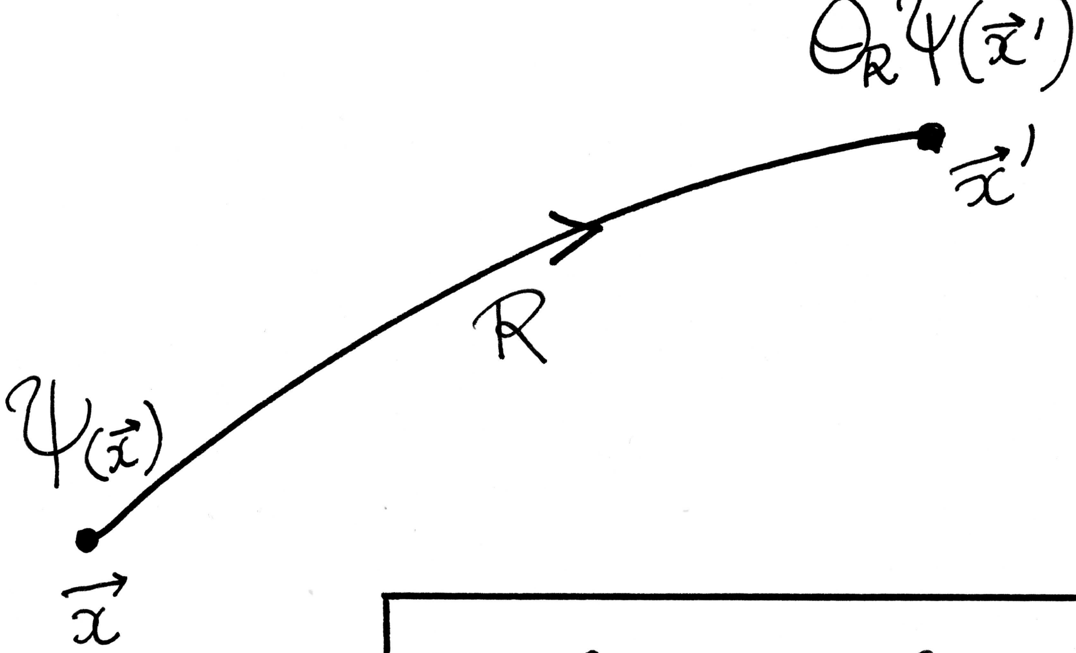


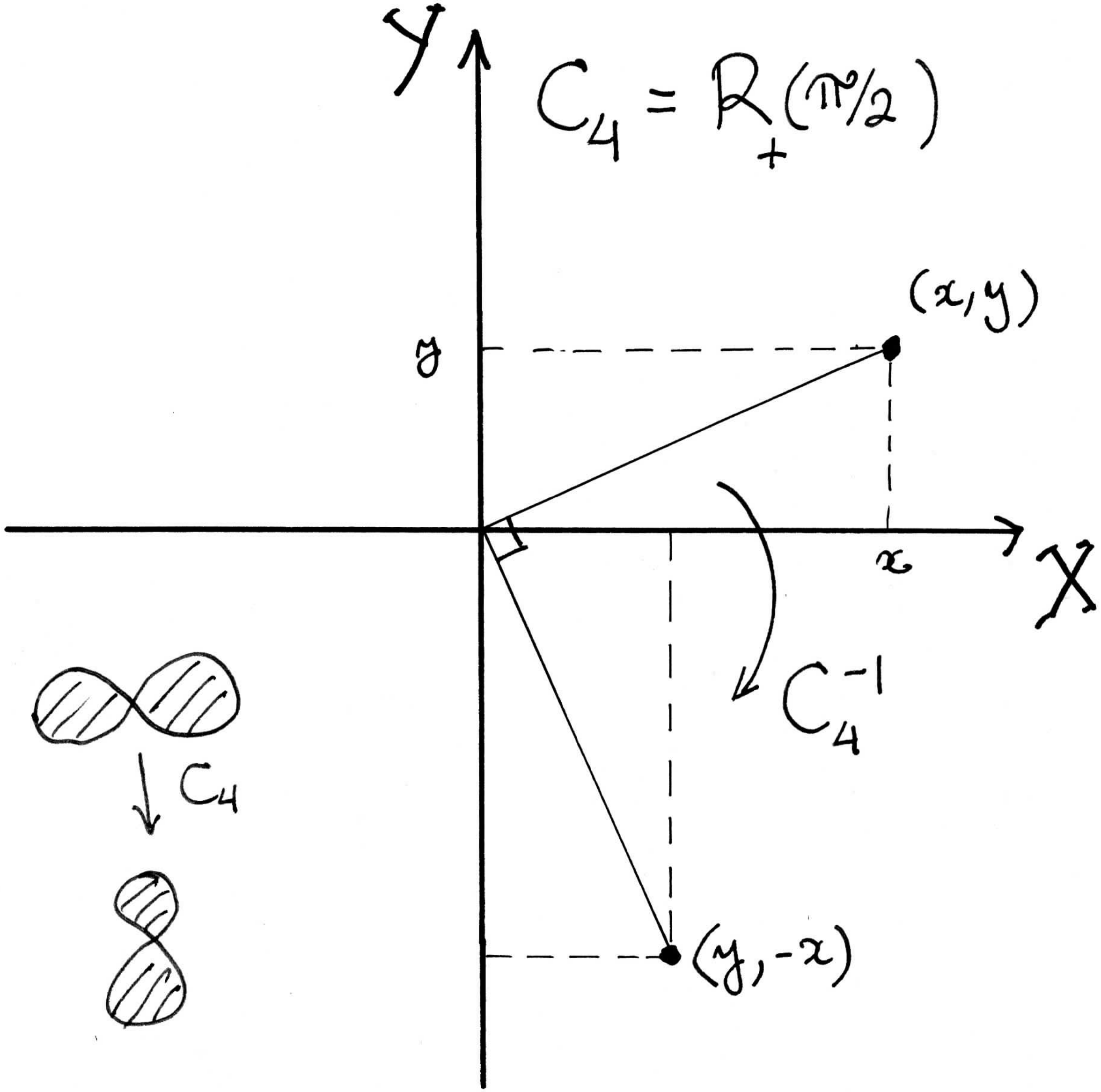
Def. (Wigner)

$$\boxed{O_R\psi(\vec{x}\,') = \psi(\vec{x})}$$

$$\Updownarrow$$

$$\boxed{O_R\psi(\vec{x}) = \psi(R^{-1}\vec{x})}$$

$C_4 = R_+(\pi/2)$



Orbital p_x:

$$\psi_{p_x}(\vec{x}) = C\, x \exp[-\lambda(x^2+y^2+z^2)]$$

Rodar a função:

$$O_{C_4}\psi_{p_x}(\vec{x}) = \psi_{p_x}(C_4^{-1}\vec{x})$$

$$= C\, y \exp[-\lambda(x^2+y^2+z^2)]$$

$$= \psi_{p_y}(\vec{x})$$

Resultado: $\boxed{O_{C_4}\psi_{p_x} = \psi_{p_y}}$,

$$C_4^{-1}(x,y,z) = (y,-x,z)$$

LEMAS DE SCHUR

Lema I

$\Gamma(a)$ rep. de G, $a \in G$

$\exists$ M, tal que

$$\boxed{M\Gamma(a) = \Gamma(a)M, \ \forall a \in G}$$

i) Γ é RI $\Rightarrow M = c \cdot 1$;

ii) $M \neq c \cdot 1 \Rightarrow \Gamma$ é RR,

Lema II

$\Gamma^{(i)}$ e $\Gamma^{(j)}$ RI's de G

$\exists$ M retangular, tal que

$$\boxed{M\Gamma^{(i)}(a) = \Gamma^{(j)}(a)M, \ \forall a \in G.}$$

i) Se $n_i \neq n_j \Rightarrow M \equiv 0$;

ii) $n_i = n_j$,

$\begin{cases} \text{ou } M \equiv 0, \\ \text{ou } M \neq 0 \Rightarrow \det M \neq 0 \end{cases}$

$\Rightarrow \quad \Gamma^{(j)}(a) = M \cdot \Gamma^{(i)}(a) \cdot M^{-1}$

equivalentes

Grande Teorema de Ortogonalidade (GTO)

$\Gamma^{(i)}, \Gamma^{(j)}$: RI's, unitárias, <u>não-equivalentes ou idênticas</u>

$$\boxed{\sum_{a \in G} \Gamma^{(i)*}_{\alpha\beta}(a)\, \Gamma^{(j)}_{\lambda\mu}(a) = \frac{h}{n_i}\,\delta_{ij}\,\delta_{\alpha\lambda}\,\delta_{\beta\mu}}$$

$n_i = \dim \Gamma^{(i)}$, $\alpha,\beta = 1,2,\dots,n_i$; $\lambda,\mu = 1,2,\dots,n_j$

$n_j = \dim \Gamma^{(j)}$

h : ordem de G

Grande Teorema de Ortogonalidade

$$v^{(j)}_{\lambda\mu}(g_k) = \Gamma^{(j)}_{\lambda\mu}(g_k) \quad , \quad k=1,2,\dots,h$$

Dimensão do espaço linear : h

Quantos vetores ortogonais ?

$\lambda,\mu = 1,2,\dots,n_j \longrightarrow$ em total n_j^2 componentes

$j=1,2,\dots,N_I \qquad N_I$: número de RI's

$$\boxed{\sum_{j\in RI} n_j^2 \leq h}$$

Caratéres, $\chi(g)$

Def.

$$\chi(g) \equiv \mathrm{Tr}\,\Gamma(g) = \sum_{\alpha} \Gamma_{\alpha\alpha}(g)$$

RI's:

$$\Gamma^{(i)}(g) \xrightarrow{\mathrm{Tr}} \chi^{(i)}(g) \xrightarrow{\mathcal{C}_\mu} \chi^{(i)}_\mu$$

Rep.'s equivalentes: $\Gamma'(g) = M \cdot \Gamma(g) \cdot M^{-1}$, $\forall g \in G$.

$$\chi'(g) = \chi(g)$$

$$\chi'_\mu = \chi_\mu \text{ , para } \mathcal{C}_\mu$$

Relações de Ortogonalidade para os Caracteres

ROC : $$\sum_{\mathcal{C}_\mu}^{N_{\mathcal{C}_\mu}} g_{\mathcal{C}_\mu} \chi_\mu^{(i)*} \chi_\mu^{(j)} = h\,\delta_{ij} \; ;$$

TEO : $$\sum_{i \in RI}^{N_I} \chi_\mu^{(i)*} \chi_\lambda^{(i)} = \frac{h}{g_{\mathcal{C}_\mu}} \delta_{\lambda\mu}$$

$N_{\mathcal{C}_\mu}$: # de classes do grupo G ; N_I : # de RI's de G.

h : ordem de G ; $g_{\mathcal{C}_\mu}$: # de elementos na classe $\mathcal{C}_\mu$

$$\Longrightarrow \quad \boxed{N_{\mathcal{C}_\mu} = N_I}$$

Redutibilidade:

$$\Gamma(g) = \sum_{i \in RI} a_i \, \Gamma^{(i)}(g) \quad , \forall g \in G$$

a_i : # de vezes que $\Gamma^{(i)}$ está contida em Γ (contando as iguais + equivalentes)

Ortogonalidade:

$$\boxed{a_i = \frac{1}{h} \sum_{\mathcal{C}_\mu} g_{\mathcal{C}_\mu} \chi_\mu \chi_\mu^{(i)*}}$$

$$\chi_\mu = Tr\left[\Gamma(g)\right]_{\mathcal{C}_\mu}$$

Teorema Célebre (Rep. Regular, Γ_R)

$$\Gamma_R = \sum_{j \in RI} n_j \, \Gamma^{(i)}$$

$\dim \Gamma_R = h$

$\dim \Gamma_j = n_j$

$$\Downarrow$$

$$\boxed{\sum_{j \in RI} n_j^2 = h}$$

$$\chi_R(g) = \begin{cases} h, & g \equiv e \\ 0, & g \neq e \end{cases}$$

C_{3v} , $h = 6$

$\mathcal{C}_\mu$:	$\{E\}$,	$\{2C_3\}$,	$\{3\sigma_v\}$
$g\mathcal{C}_\mu$:	1	2	3
RI :	Γ_1	Γ_2	Γ_3
	A	B	E
dim	1	1	2

Representação Regular:

$$\Gamma_R = 1 \cdot A + 1 \cdot B + 2 \cdot E$$

Teorema Célebre:

$$1^2 + 1^2 + 2^2 = 6$$

Idêntica

χ	$\{E\}$	$\{2C_3\}$	$\{3\sigma_v\}$
A	1	1	1
B	1	x	y
E	2	-1	0

E é ortogonal a A (ROC):

$$1 \cdot (1 \cdot 2) + 2[1 \cdot (-1)] + 3(1 \cdot 0) = 0$$

Para E:

$$1 \cdot 2^2 + 2 \cdot (-1)^2 + 3(0^2) = 6 = h$$

Para B: $1 + x - 2 = 0 \Rightarrow x = 1$

$1 + y = 0 \Rightarrow y = -1$

Álgebra

Carateres de Dirac :

$$\boxed{\Omega_{\mathcal{C}_\mu} = \sum_{T \in \mathcal{C}_\mu} T ,}$$

$\mathcal{C}_\mu$: classe conjugada

$$M^{(i)}_{\mathcal{C}_\mu} = \Gamma^{(i)}(\Omega_{\mathcal{C}_\mu}) = \sum_{R \in \mathcal{C}_\mu} \Gamma^{(i)}(R) = \lambda^{(i)}_\mu \cdot \mathbb{1}$$

$$\boxed{\lambda^{(i)}_\mu = \frac{g_{\mathcal{C}_\mu}}{n_i} \chi^{(i)}_\mu}$$

$$\Omega_{\mathcal{C}_\lambda}\,\Omega_{\mathcal{C}_\mu} = \sum_\sigma c_{\lambda\mu\sigma}\,\Omega_{\mathcal{C}_\sigma}$$

$$c_{\lambda\mu\sigma} = c_{\mu\lambda\sigma}$$

Álgebra para os carateres:

$$g_{\mathcal{C}_\lambda}\, g_{\mathcal{C}_\mu}\, \chi^{(i)}_\lambda\, \chi^{(i)}_\mu = n_i \sum_\sigma c_{\lambda\mu\sigma}\, g_{\mathcal{C}_\sigma}\, \chi^{(i)}_\sigma$$

Projetores

$$\boxed{P_{\lambda}^{(j)} = \frac{n_j}{h} \sum_{R \in G} \Gamma_{\lambda\lambda}^{(j)*}(R)\, \Theta_R}$$

$$P_{\lambda}^{(j)} \psi_{\alpha}^{(i)} = \delta_{ij}\, \delta_{\lambda\alpha}\, \psi_{\lambda}^{(j)}$$

Projeta sobre a variedade $\mathcal{L}^{(j)}$:

$$\boxed{P^{(j)} = \sum_{\lambda} P_{\lambda}^{(j)} = \frac{n_j}{h} \sum_{R \in G} \chi^{(j)*}(R)\, \Theta_R}$$