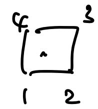
HW. <u>P30.</u>



$$D_4 = \langle r, s \mid r^4 = s^2 = (rs)^2 = 1 \rangle$$

$r = (1234)$

$s = (12)(34)$

$$= \langle 1, r, r^2, r^3, s, rs, r^2 s, r^3 s$$

$rs = sr^3$, $r^2 s = sr^2$, $r^3 s = sr$

$(rs)^2 = 1$

$$rs = sr^3 \iff s^{-1} r^{-1} = sr^3$$

$$\iff 1 = s^2 r^4 = 1 \quad \checkmark$$

$$D_4 = \{1\} \cup \{r, r^3\} \cup \{r^2\} \cup \{s, r^2 s\} \cup \{rs, r^3 s\}$$

$$s\underline{rs} = s \cdot s^{-1} \cdot r^{-1} = r^{-1} = r^3$$

$$=: \underset{1}{[1]} \cup \underset{2}{[r]} \cup \underset{3}{[r^2]} \cup \underset{4}{[s]} \cup \underset{5}{[rs]}$$

$C_1 = 1$, $C_2 = r + r^3$, $C_3 = r^2$, $C_4 = s + r^2 s$, $C_5 = rs + r^3 s$

	C_1	C_2	C_3	C_4	C_5
C_1	C_1	C_2	C_3	C_4	C_5
C_2		$2C_1 + 2C_3$			
C_3					
C_4					
C_5					

$$C_2 \cdot C_2 = (r + r^3)(r + r^3) = r^2 + r^4 + r^4 + r^6 = 2 + 2r^2$$

$$= 2C_1 + 2C_3$$

Character table for point group D_4

1 r r^2 s rs

D_4	E	$2C_4$ (z)	C_2 (z)	$2C'_2$	$2C''_2$	linear functions, rotations	quadratic functions	cubic functions
A_1	+1	+1	+1	+1	+1	-	x^2+y^2, z^2	-
A_2	+1	+1	+1	-1	-1	z, R_z	-	z^3, $z(x^2+y^2)$
B_1	+1	-1	+1	+1	-1	-	x^2-y^2	xyz
B_2	+1	-1	+1	-1	+1	-	xy	$z(x^2-y^2)$
E	+2	0	-2	0	0	(x, y) (R_x, R_y)	(xz, yz)	(xz^2, yz^2) (xy^2, x^2y) (x^3, y^3)

Mulliken symbols:

A / B : 1D irreps. symmetric/antisymmetric w.r.t. principle rotation axis.

$\chi(C_n) = \pm 1$

E 2D "entartet". degenerate

T 3D

G 4D

H 5D

---

subscript.

1/2 : symm / antisymm. w.r.t. vertical mirror plane

g/u : "Eg / t2g" gerade / ungerade
even/ odd.

inversion $\chi(i) = \pm 1$

' / '' : sym / antsym. w.r.t. σ_h

Characters of irreps of SO(3), SU(2)

Conjugacy classes labeled by rotation angle θ around some axes

$$R = e^{i\theta \hat{n}\cdot\hat{J}} \sim R_z = e^{i\theta J_z}$$

$$J_z = \mathrm{diag}(j, j-1, \cdots -j)$$

$$\chi^j(\theta) = \mathrm{Tr}\,\mathrm{diag}(e^{i\theta j}, e^{i\theta(j-1)} \cdots e^{-i\theta j})$$

$$= e^{i\theta j}\frac{1-e^{-i(2j+1)\theta}}{1-e^{-i\theta}} = \boxed{\frac{\sin(j+\frac{1}{2})\theta}{\sin\frac{\theta}{2}}}$$

Haar measure $\frac{1}{\pi}\int_0^{2\pi}\sin^2\frac{\theta}{2}\,d\theta$

$$= \frac{1}{2\pi}\int_0^{2\pi}(1-\cos\theta)\,d\theta$$

$$\langle \chi^j, \chi^{j'}\rangle = \delta_{jj'}$$

$$V^{j_1}\otimes V^{j_2} \simeq \bigoplus_{j=|j_1-j_2|}^{j_1+j_2} V^j$$

$$\chi_{j_1\otimes j_2} = \chi_{j_1}\cdot\chi_{j_2} = \sum_{|j_1-j_2|}^{j_1+j_2}\chi^j$$

$\langle \chi_j, \chi_{j_1}\chi_{j_2}\rangle = 1$ iff $|j_1-j_2|\le j\le j_1+j_2$

$$V^{\frac{1}{2}}\otimes V^{\frac{1}{2}} \simeq V^0\oplus V^1$$

$j \quad m \qquad\qquad\qquad\qquad\qquad J \quad M$

$|\tfrac{1}{2}, \pm\tfrac{1}{2}\rangle \otimes |\tfrac{1}{2}, \pm\tfrac{1}{2}\rangle \rightarrow |0, 0\rangle$

$|1, \pm 1\rangle, \; |1, 0\rangle$

CG - coefficient $\langle \underline{j_1 m_1 ; j_2 m_2} | \underline{J, M} \rangle$

Application of group representations.

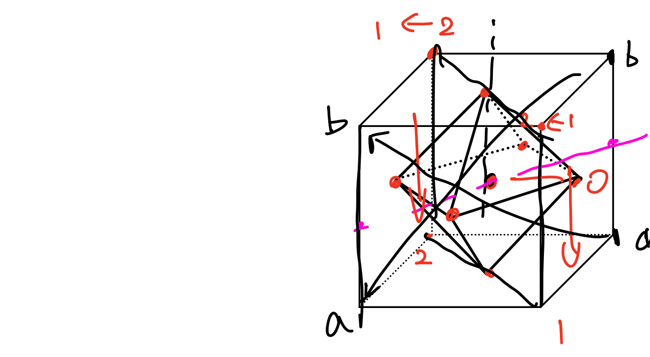
(Dresselhaus . Group Theory)

- $\underset{\sim}{O(3)}$ $\qquad O(3) \overset{\sim}{=} SO(3) \times \mathbb{Z}_2$

$\downarrow$ embed in a crystal $\qquad \downarrow$ V^j is irrep of $O(3)$

$O(3) \rightarrow$ PG. $\qquad V^j = \mathrm{span}\{Y_{lm}\}$

$\underline{(-1)^l}$



perovskite structure

Cu . oxides

$d \longrightarrow$?

Point group $O_h \subset O(3)$

$\underline{24}$ $\quad E$; $8C_3$; $3C_2$; $6C_2'$; $6C_4$ $\subset SO(3)$

(body diagonal)

Couple with inversion

24 $\quad I \ ; \ 8S_6 = I\cdot C_3 \ ; \ 3\underline{\sigma_h} = I C_2 \ ; \ 6\underline{\sigma_d} = \underline{I\cdot C_2'}$

σ_h : mirror $\perp$ principle rot. axis

σ_d : diag. plane

$|O_h| = 48$

O_h	E	$8C_3$	$6C_2$	$6C_4$	$3C_2 = (C_4)^2$	i	$6S_4$	$8S_6$	$3\sigma_h$	$6\sigma_d$	linear functions, rotations	quadratic functions	cubic functions
A_{1g}	+1	+1	+1	+1	+1	+1	+1	+1	+1	+1	-	$x^2+y^2+z^2$	-
A_{2g}	+1	+1	-1	-1	+1	+1	-1	+1	+1	-1	-	-	-
E_g	+2	-1	0	0	+2	+2	0	-1	+2	0	-	$(2z^2-x^2-y^2, x^2-y^2)$	-
T_{1g}	+3	0	-1	+1	-1	+3	+1	0	-1	-1	(R_x, R_y, R_z)	-	-
T_{2g}	+3	0	+1	-1	-1	+3	-1	0	-1	+1	-	(xz, yz, xy)	-
A_{1u}	+1	+1	+1	+1	+1	-1	-1	-1	-1	-1	-	-	-
A_{2u}	+1	+1	-1	-1	+1	-1	+1	-1	-1	+1	-	-	xyz
E_u	+2	-1	0	0	+2	-2	0	+1	-2	0	-	-	-
T_{1u}	+3	0	-1	+1	-1	-3	-1	0	+1	+1	(x, y, z)	-	(x^3, y^3, z^3) $[x(z^2+y^2), y(z^2+x^2), z(x^2+y^2)]$
T_{2u}	+3	0	+1	-1	-1	-3	+1	0	+1	-1	-	-	$[x(z^2-y^2), y(z^2-x^2), z(x^2-y^2)]$

g: $\rho(I) = 1$

u: $\rho(I) = -1$

$$\chi(\theta) = \frac{\sin(l+\frac{1}{2})\theta}{\sin\frac{\theta}{2}}$$

	dim	irreps of Oh
① s orbital $l=0$	1	A_{1g}
② $\underline{p}$ orbital $l=1$	3 $\rightarrow$	$\underline{T_{1u}}$

	E	$8C_3$	$3C_2$	$6C_2'$	$6C_4$
χ:	3	$\frac{\sin\frac{3}{2}\cdot\frac{2}{3}\pi}{\sin\frac{1}{3}\pi} = 0$	$\frac{\sin\frac{3}{2}\cdot\pi}{\sin\frac{\pi}{2}} = -1$	-1	1
$I($	-3	0	1	1	$-1)$

6

$$\langle \chi, \chi \rangle = \frac{2(9+3+6+6)}{48} = 1$$

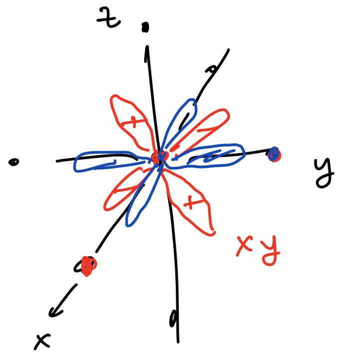
③ d orbital $\quad l=2 \quad 5 \quad \underline{E_g + T_{2g}}$

④ f $\quad l=3 \quad 7 \quad A_{2u} + T_{1u} + T_{2u}$

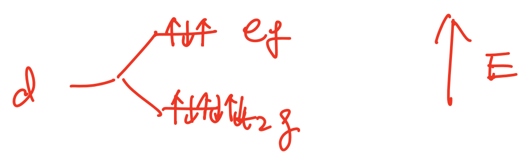
$\qquad\qquad\qquad\qquad\qquad\qquad 1 + 3 + 3$

$$d \xrightarrow{O_h} e_g + t_{2g}$$

e_g : $\begin{cases} 3z^2-1 \\ x^2-y^2 \end{cases}$



t_{2g} : $\begin{cases} xy \\ yz \\ zx \end{cases}$ $\sim \begin{cases} z \\ x \\ y \end{cases}$ "p"



Cu^{2+} : d^9

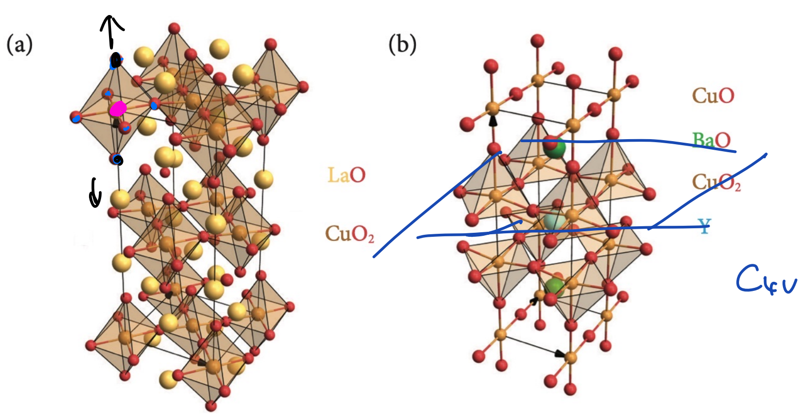
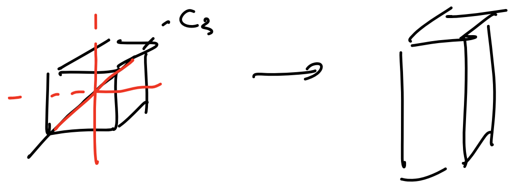


Figure 2.8 | Structures of (a) La_2CuO_4 and (b) $YBa_2Cu_3O_7$.

tetragonal

7



Character table for point group D_{4h}

(x axis coincident with C'_2 axis)

D_{4h}	E	$2C_4$ (z)	C_2	$2C'_2$	$2C''_2$	i	$2S_4$	σ_h	$2\sigma_v$	$2\sigma_d$	linear functions, rotations	quadratic functions	cubic functions
A_{1g}	+1	+1	+1	+1	+1	+1	+1	+1	+1	+1	-	x^2+y^2, z^2	-
A_{2g}	+1	+1	+1	-1	-1	+1	+1	+1	-1	-1	R_z	-	-
B_{1g}	+1	-1	+1	+1	-1	+1	-1	+1	+1	-1	-	x^2-y^2	-
B_{2g}	+1	-1	+1	-1	+1	+1	-1	+1	-1	+1	-	xy	-
E_g	+2	0	-2	0	0	+2	0	-2	0	0	(R_x, R_y)	(xz, yz)	
A_{1u}	+1	+1	+1	+1	+1	-1	-1	-1	-1	-1	-	-	-
A_{2u}	+1	+1	+1	-1	-1	-1	-1	-1	+1	+1	z	-	$z^3, z(x^2+y^2)$
B_{1u}	+1	-1	+1	+1	-1	-1	+1	-1	-1	+1	-	-	xyz
B_{2u}	+1	-1	+1	-1	+1	-1	+1	-1	+1	-1	-	-	$z(x^2-y^2)$
E_u	+2	0	-2	0	0	-2	0	+2	0	0	(x, y)	-	(xz^2, yz^2) (xy^2, x^2y), (x^3, y^3)

g

u

O_h $\tilde{E}_g$ 2 0 2 2 0

$\tilde{T}_{2g}$ 3 1 -1 -1 -1

$$a_{b_1g} = \langle \chi_{b_1g} \cdot \chi_{\tilde{E}_g} \rangle = 1$$

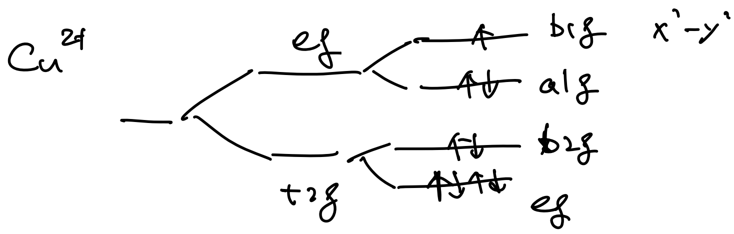
$$O_h \longrightarrow D_{4h}$$

$$E_g \longrightarrow A_{1g} + B_{1g}$$

$3z^2-1,\ x^2-y^2$ $\qquad$ $\underline{3z^2-1}$ $\quad$ x^2-y^2

$$T_{2g} \longrightarrow E_g + B_{2g}$$

$xy/yz/xz$ $\qquad$ $\underline{yz/xz}$ $\quad$ xy



Cuprate superconductors. only active orbital is big $= x^2-y^2$

— selection rules of dipole transitions.

$$H_{int} = \frac{(\vec{p}+e\vec{A})^2}{2m} - \frac{\vec{p}^{\,2}}{2m} = \frac{e}{m}\vec{p}\cdot\vec{A} + \cancel{\frac{e^2}{2m}\vec{A}^2}$$

(coulomb gauge $\nabla\cdot A = 0$)

$$A(\vec{r}) \propto \vec{\epsilon}\cdot a_{k\epsilon}\, e^{i\vec{k}\cdot\vec{r}} + h.c.$$

→ photon operators

$$\Rightarrow H_{int} \simeq \vec{\epsilon}\cdot\vec{p}$$

$$W \propto |\langle f|H_{int}|i\rangle|^2 \delta(E_f - E_i)$$

$$\langle f|H_{int}|i\rangle \propto \vec{\epsilon}\cdot\langle f|\vec{p}|i\rangle$$

$$\propto \vec{e}\cdot\langle f|[H,\vec{r}]|i\rangle$$

$$\langle f|\hat{H}\vec{r}-\vec{r}\hat{H}|i\rangle$$

$$\propto (E_f - E_i)\langle f|\vec{r}|i\rangle$$

$$\langle f|\vec{r}|i\rangle \propto \langle l'm'|Y^{l=1}_{q}(\hat{r})|lm\rangle$$

$q = 0, \pm 1$

3j symbol $\begin{array}{c} l \\ m \end{array} \propto \underbrace{\begin{pmatrix} l' & 1 & l \\ -m' & q & m \end{pmatrix}}_{A} \underbrace{\begin{pmatrix} l' & 1 & l \\ 0 & 0 & 0 \end{pmatrix}}_{B}$

selection rules: $\sum m_i = 0$

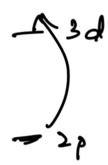
$$\begin{cases} A: \quad -m' + q + m = 0 \\ \quad |l' - l| \le 1 \end{cases}$$

B: $\forall m = 0$. $l' + l + l =$ even.

$\Rightarrow$ dipole transition selection rule:

$$\begin{cases} \Delta l = \pm 1 \\ \Delta m = 0, \pm 1 \end{cases}$$

Cu: $2p \longrightarrow 3d$



$l = 2 \quad m = \pm 2$

$d_{x^2-y^2} = \frac{1}{\sqrt{2}} (Y_{2,2} + Y_{2,-2})$

$$A. \quad \begin{array}{ccc} d & & p \\ \hline \end{array}$$

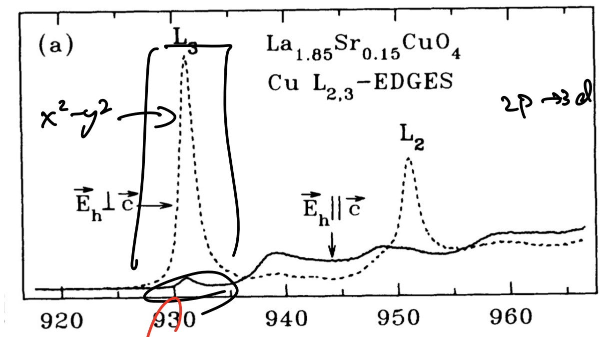
$$A. \begin{pmatrix} l' & 1 & l=1 \\ -m' & q & m \end{pmatrix} \neq 0$$

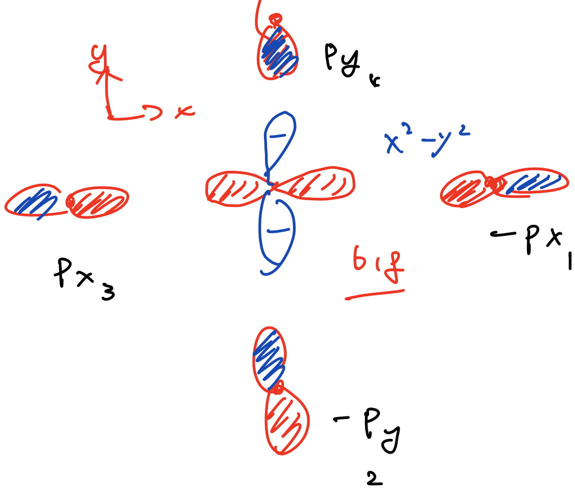
$m' = \pm 2 \quad |q| \le 1 \quad |m| \le 1$

$q = \pm 1 \quad m = 1$

$q = \pm 1$: $\vec{E}, \vec{r} \parallel x, y$ ✓

$\vec{E}, \vec{r} \parallel z$, $m = 0$





$$\frac{1}{2}\left(-p_{x_1} - p_{y_2} + p_{x_3} + p_{y_4}\right)$$

$\sim b_{1g}$

$d - p$

"Zhang-rice singlet"

Zhang & Rice

PRB 37, 3759 (R) (1988)