$\underline{\text{Recap}}$ (Induced) rep of SU(2)

$V \rightsquigarrow H \subset G.$

$$\mathrm{Ind}_H^G V = \{ \Psi : \underline{G} \longrightarrow \underline{V} \mid \Psi(gh^{-1}) = \rho_V(h)\Psi(g), \forall h \in H, g \in G \}$$

$$H = D = \begin{pmatrix} \alpha & 0 \\ 0 & \bar{\alpha} \end{pmatrix} \cong U(1)$$

$$\mathrm{Ind}_{U(1)}^{SU(2)} V = \mathrm{span}\{ \underline{\Psi(ue^{i\theta}, ve^{i\theta}) = e^{ik\theta}\Psi(u,v)} \}$$

$$|u|^2 + |v|^2 = 1$$

$$\rho_{\underset{\mathbb{Z}}{k}}(\theta) = e^{ik\theta} \qquad (\widehat{U(1)} = \mathbb{Z})$$

restrict to $\underline{\text{holomorphic}}$ functions

$\hookrightarrow$ homogeneous polynomials

$$\underline{\mathcal{H}_k} = \mathrm{span}\{ \underset{\Delta}{u^k}, u^{k-1}v, \ldots, uv^{k-1}, v^k \} \ni \Psi$$

$$(g\Psi) \in \mathcal{H}_k$$

$$\hookrightarrow \mathcal{H}_k \cong V_j := \mathrm{span}\{ \underline{\tilde{f}_{j,m}}(u,v) = u^{j+m} v^{j-m}$$

$$m = -j, -j+1, \ldots, j \}$$

$$\# m = 2j+1$$

$$(g\cdot\tilde{f}_{j,m})(u,v) = \tilde{f}(\bar{\alpha}u+\bar{\beta}v,\ -\beta u+\alpha v)$$

$$= \underline{(\bar{\alpha}u+\bar{\beta}v)^{j+m}(-\beta u+\alpha v)^{j-m}}$$

$$=: \sum_{m'} \underline{\tilde{D}^{j}_{m'm}}(g)\, \underline{\tilde{f}_{j,m'}(u,v)}$$

$$\underline{\tilde{D}^{j}_{m',-j}(g)} \propto \tilde{f}_{j,-m'}(\alpha,\beta)$$

$$\underline{g\in D} \Rightarrow \underline{\tilde{D}^{j}_{m'm} = \alpha^{-2m}\,\delta_{m'm}}$$

$(\hat{J}_z \quad |j,m\rangle$ diagonal $)$

$$SO(3) \cong SU(2)/\mathbb{Z}_2$$

$$\begin{tikzcd} SU(2) \arrow[r, "\pi"] \arrow[d, "\tilde{\rho}"'] & SO(3) \arrow[dl, "\rho"] \\ GL(V) & \end{tikzcd}$$

$(\pi(U)=\pi(-U))$

$$\tilde{\rho} = \rho\circ\pi$$

$$\pi(-1) = 1$$

$\underline{m = -j, -j+1 \dots j}$

$$\tilde{\rho}(-1) = \rho\circ\pi(-1) = \rho(1) = 1$$

$$g=\begin{pmatrix}-1 & 0\\ 0 & -1\end{pmatrix} \Rightarrow (-1)^{-2m} = 1$$

$m \in$ integer

$\rightarrow$ $\underline{j \in \text{integer.}}$

$$g \sim d(z) = \underline{\begin{pmatrix} z & 0 \\ 0 & z^{-1} \end{pmatrix}} \qquad |z| = 1$$

$$\chi_j(g) = \sum_{m=-j}^{j} z^{-2m} = \frac{z^{2j+1} - z^{-2j-1}}{z - z^{-1}}$$

$$\hookrightarrow \quad \langle \chi_j , \chi_{j'} \rangle = \underline{\delta_{jj'}}$$

$$\langle \chi_j , \chi_j \rangle = 1 \Rightarrow \underline{V_j \text{ irrep}}$$

---

①

- $\underline{\text{Unitarization}}$

$$\hat{f}_{j,m} \propto \underline{u^{j+m}}\, \underline{v^{j-m}}$$

$$\langle f , g \rangle = \underline{\frac{1}{\pi (2j+1)!}} \int_{\mathbb{C}^2} \bar{f} \cdot g \; e^{-(|u|^2 + |v|^2)} \, du \, d\bar{u} \, dv \, d\bar{v}$$

$$\hookrightarrow \quad f_{j,m} = \frac{1}{\sqrt{\pi}} \sqrt{\frac{(2j+1)!}{(j+m)!(j-m)!}} \; u^{j+m} v^{j-m}$$

$$\hookrightarrow \quad \underline{D^{j}_{m,0}} = \underline{Y_{\ell m}(\theta , \phi)}$$

- <u>tensor products</u> : Clebsch-Gordon decomposition

<u>Check</u> $\underline{V_{j_1} \otimes V_{j_2} \cong V_{|j_1-j_2|} \oplus V_{|j_1-j_2|+1} \oplus \cdots \oplus V_{j_1+j_2}}$

$$\underline{V_{\frac{1}{2}} \otimes V_j \cong V_{j-\frac{1}{2}} \oplus V_{j+\frac{1}{2}}}$$

$$\chi_j = \frac{z^{2j+1} - z^{-2j-1}}{z - z^{-1}}$$

$$\chi_{\frac{1}{2}}(z)\chi_j(z) = (z + z^{-1}) \frac{z^{2j+1} - z^{-2j-1}}{z - z^{-1}}$$

$$= \chi_{j+\frac{1}{2}} + \chi_{j-\frac{1}{2}}$$

<u>Check.</u> $\langle \chi_{j_1}\chi_{j_2}, \chi_j \rangle = 1$ iff $|j_1-j_2| \le j \le j_1+j_2$

$$\underline{P^j_{m'm} = \int_{SU(2)} \overline{D^j_{m'm}(g)}\, T(g)\, dg}$$

For the <u>trivial rep.</u> $\quad P^0 = \int T(g)\, dg$

$$T(g)\left(|\underline{\beta}\rangle \otimes |\underline{\delta}\rangle\right) := \underline{g_{\alpha\beta}}\, \underline{g_{\gamma\delta}}\left(|\alpha\rangle \otimes |\gamma\rangle\right)$$

$$\int g_{\alpha\beta}\, g_{\gamma\delta}\, dg = \frac{1}{2}\epsilon_{\alpha\gamma}\epsilon_{\beta\delta} \qquad \text{(HW 2)}$$

$$\underline{\epsilon_{\alpha\gamma}}\,\epsilon_{\beta\delta}\,|\underline{\alpha}\rangle\otimes|\underline{\gamma}\rangle = \epsilon_{\beta\delta}\,(\underbrace{|\underline{+}\rangle\otimes|-\rangle - |-\rangle\otimes|+\rangle}_{\text{singlet}})$$

$$|0,0\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$$

---

$$V_{\frac{1}{2}} \otimes V_{\frac{1}{2}} = \underset{1}{V_0} \oplus \underset{3}{V_1}$$

3-dim complement:

$$\begin{cases} |1,1\rangle = |+\rangle\otimes|+\rangle \\ |1,0\rangle = \frac{1}{\sqrt{2}}(|+\rangle\otimes|-\rangle + |-\rangle\otimes|+\rangle) \\ |1,-1\rangle = |-\rangle\otimes|-\rangle \end{cases}$$

---

## Wigner – Eckart theorem:

observable $O_{j,m}$

$$\langle \underline{j_1}, m_1 | O_{j,m} | j_2, m_2\rangle = \underline{\langle j_1, \underline{m_1} | j\,\underline{m} ; j_2, \underline{m_2}\rangle} \times \underbrace{\langle j_1 \| O^j \| j_2\rangle}_{\text{reduced matrix element.}}$$

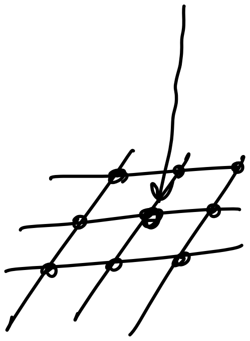
CG-coefficient / Wigner-3J symbol

important for selection rules etc

## – Application of Group rep. theory

- free ion $G = O(3)$

$\downarrow$ embedding



crystal $G = PG$.

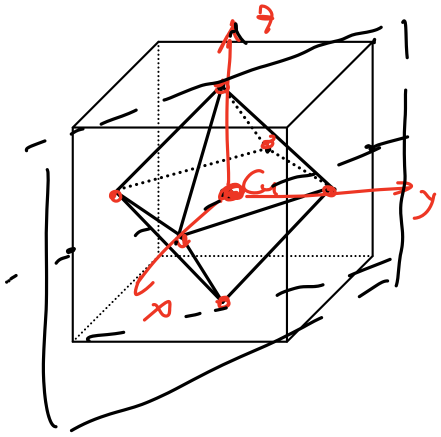
$\underline{SO(3)} \times \underline{\mathbb{Z}_2} \cong O(3)$

$(g, \pm 1) \mapsto \underline{\pm g}$

$\underline{V_j} \quad (j \in \mathbb{N})$

$V_j \cong \text{span}\{Y_{lm}\}$

$$\chi_l(\phi) = \sum_{m=-l}^{l} e^{im\phi} = \frac{\sin(l+\frac{1}{2})\phi}{\sin\frac{1}{2}\phi}$$



proper rotations $O(3) = \underline{SO(3)} \sqcup PSO(3)$

$E \,;\, 8C_3 \,;\, 3C_2 \,;\, 6C_2' : 6C_4$

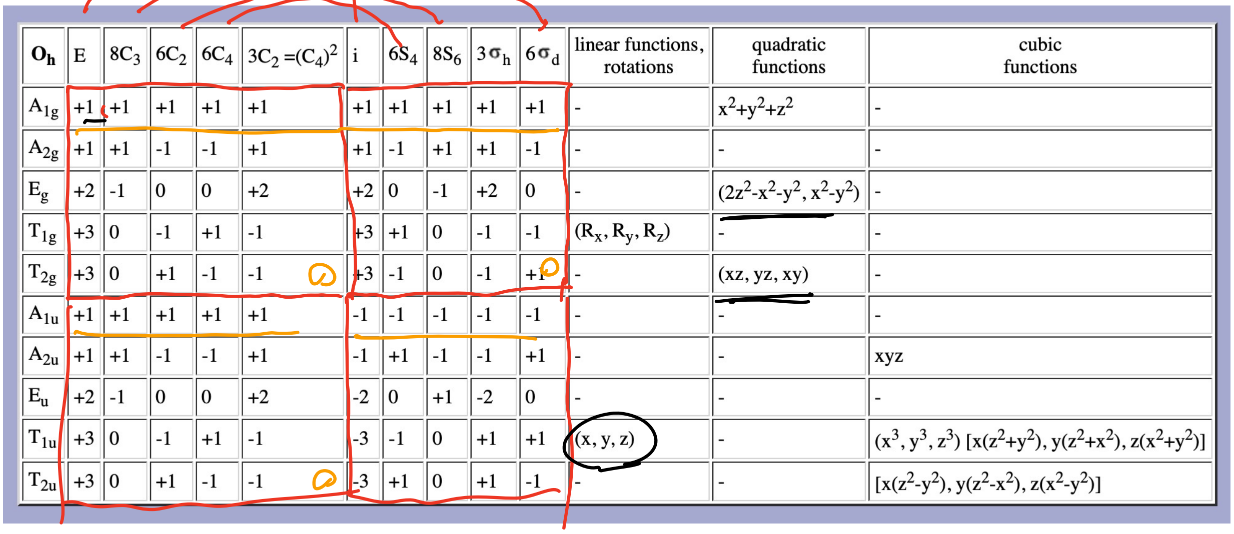
$\underline{I} \,;\, 8S_6 = IC_3 \,;\, 3\sigma_h = IC_2 \,;\, 6\sigma_d = I \cdot C_2'$

$6S_4 = IC_4$

$$\left( S_n = \sigma_h \cdot C_n = \begin{cases} I \cdot C_n & n \text{ odd} \\ I \cdot C_{n/2} & n \text{ even} \end{cases} \right)$$

$|O_h| = 48$

⑤



| $O_h$ | 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 | - | - | $[x(z^2-y^2), y(z^2-x^2), z(x^2-y^2)]$ |

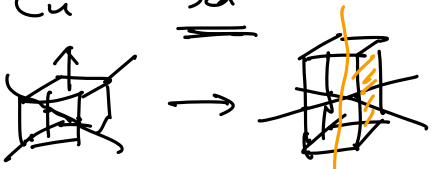
| | | | dim | irreps of Oh |
|---|---|---|---|---|
| ① s: | $l=0$ , | $Y_{00} = \frac{1}{2}\sqrt{\frac{1}{\pi}}$ | 1 | $A_{1g}$ |
| ② p: | $l=1$ | $p_{x,y,z} \propto x, y, z$ | 3 | $T_{1u}$ |

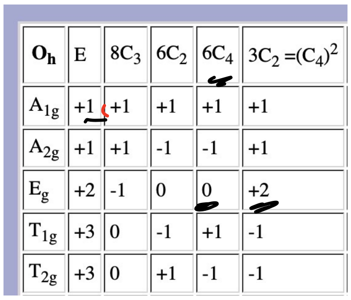
$$a_\mu = \langle \chi_\mu . \chi_l \rangle$$

| | | | |
|---|---|---|---|
| ③ d: | $l=2$ | 5 | $E_g + T_{2g}$<br>2 + 3 |
| ④ f: | $l=3$ | 7 | $A_{2u} + T_{1u} + T_{2u}$<br>1 + 3 + 3 |

---

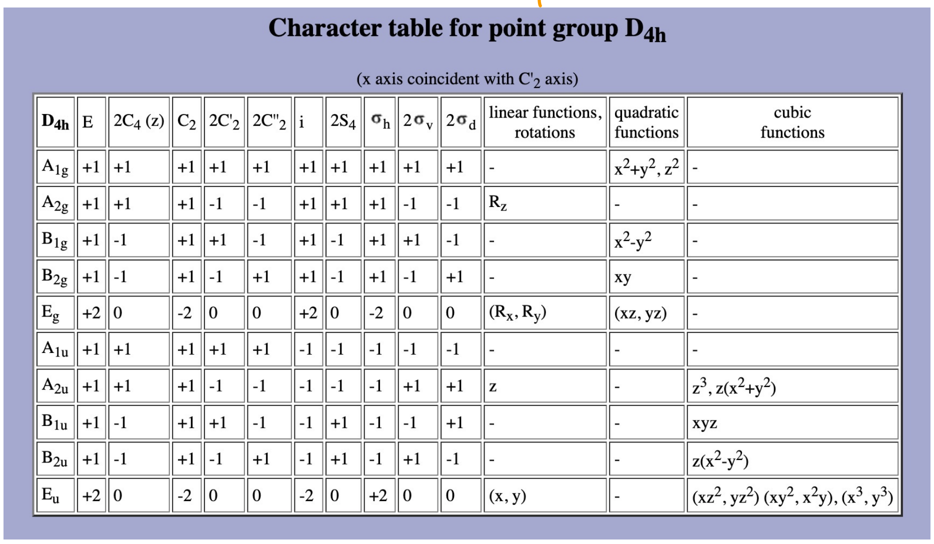
Cu : $[Ar]\,3d^{10}\,4s^1$  $Cu^{2+}$  $3d^9$





| $O_h$ | E | $8C_3$ | $6C_2$ | $6C_4$ | $3C_2 = (C_4)^2$ |
|---|---|---|---|---|---|
| $A_{1g}$ | +1 | +1 | +1 | +1 | +1 |
| $A_{2g}$ | +1 | +1 | -1 | -1 | +1 |
| $E_g$ | +2 | -1 | 0 | 0 | +2 |
| $T_{1g}$ | +3 | 0 | -1 | +1 | -1 |
| $T_{2g}$ | +3 | 0 | +1 | -1 | -1 |

$d \rightarrow E_g + T_{2g}$



## 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 | $2S_4$ | $\sigma_h$ | $2\sigma_v$ | $2\sigma_d$ | 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) | - | $(xz^2, yz^2)$ $(xy^2, x^2y)$, $(x^3, y^3)$ |

| Oh: | | |
|---|---|---|
| | $E_g$ | 2 0 2 2 0 |
| | $T_{2g}$ | 3, 1, -1, -1, -1 |

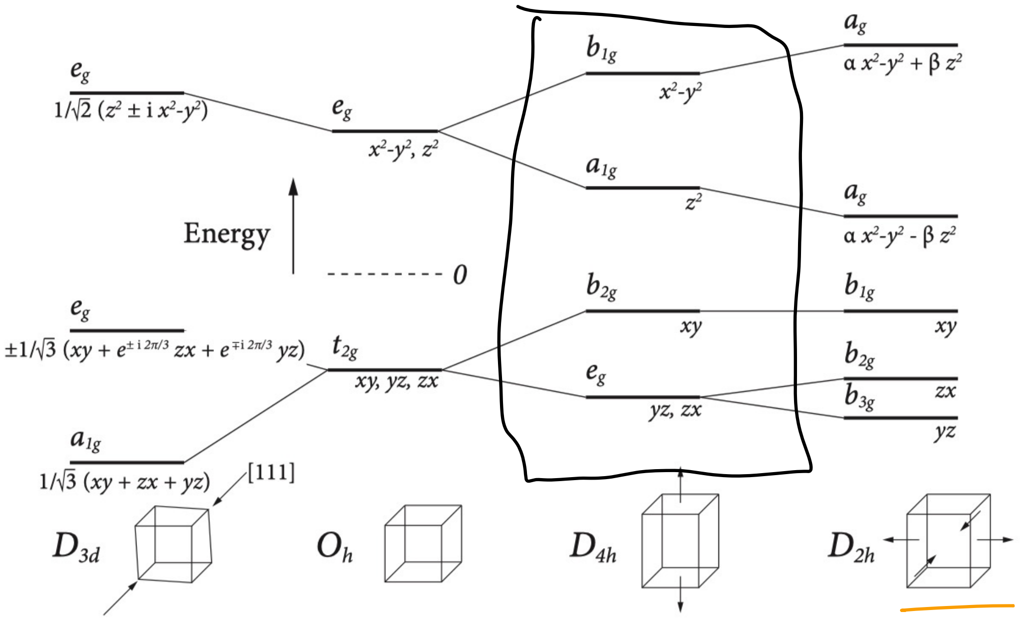
$O_h \longrightarrow D_{4h}$

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

$z^2 \qquad x^2-y^2$

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

$yz, zx \qquad xy$



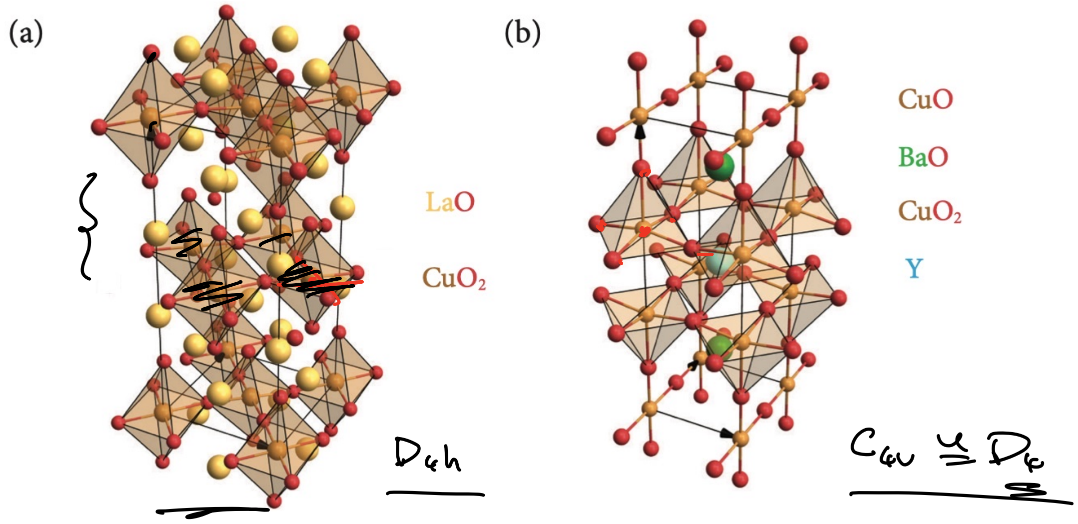
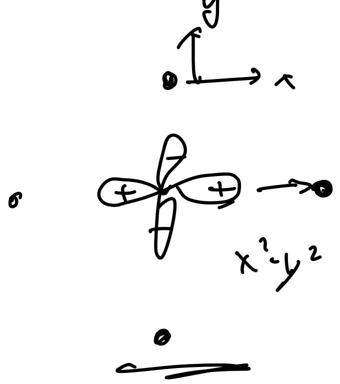
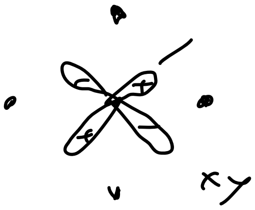


**Figure 2.8** | Structures of (a) $La_2CuO_4$ and (b) $YBa_2Cu_3O_7$.

+6 +2 -8





$Cu^{2+}$ : $d^9$

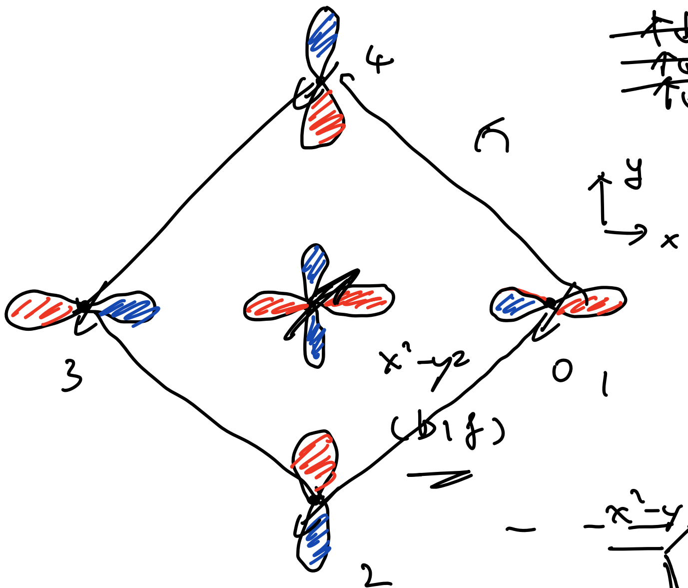
↑ $x^2-y^2$

↑↓ $z^2$

↑↓ xy, yz, zx

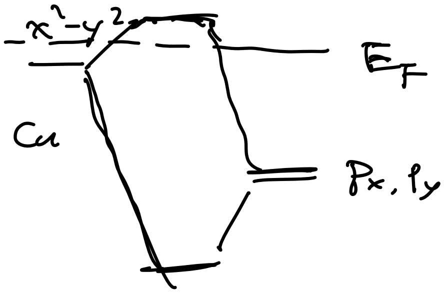
↑↓

↑↓



O : $P_x$, $P_y$

$$\mu = \frac{1}{2}(P_{1x} + P_{2y} - P_{3x} - P_{4y})$$



"Zhang-rice" singlet (PRB 37, 3759 (R) (1988))

"Simplest" model for High-$T_c$

$$H = -t \sum_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

# How to verify the low-energy model?

Light-matter interaction:

$$\vec{P} \longrightarrow \vec{P} + e\vec{A}$$

$$\underline{H_{Int}} = \frac{(\vec{P}+e\vec{A})^2}{2m} - \frac{\vec{P}^2}{2m} \approx \frac{e}{m}\vec{P}\cdot\vec{A}$$

$$\approx \underline{\vec{E}\cdot\vec{P}} \qquad \underline{\vec{P}\propto\vec{r}}$$

$$w = \underline{|\langle \underline{f}|H_{Int}|\underline{i}\rangle|^2}\,\delta(E_f - E_i)$$

$$\langle f|\underline{\vec{r}}|i\rangle \propto \langle l'm'|\underline{Y_q^1}(\hat{r})|lm\rangle$$

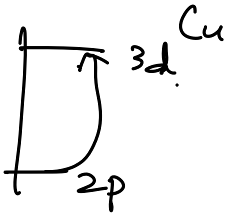
$$\propto \underbrace{\begin{pmatrix} l' & 1 & l \\ -m' & q & m \end{pmatrix}}_{A} \underline{\langle l'\|Y^1\|l\rangle} \hookrightarrow \underbrace{\begin{pmatrix} l' & 1 & l \\ 0 & 0 & 0 \end{pmatrix}}_{B}$$

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

$$B. \quad l'+l+1 = \text{even}$$

<u>dipole</u> selection rules: $\underline{\begin{cases} \Delta l = \pm 1 \\ \Delta m = 0, \pm 1 \end{cases}}$

X-ray absorption.



$$d_{x^2-y^2} = \frac{1}{\sqrt{2}}\left(Y_2^{-2} + Y_2^{2}\right) \qquad l=2$$

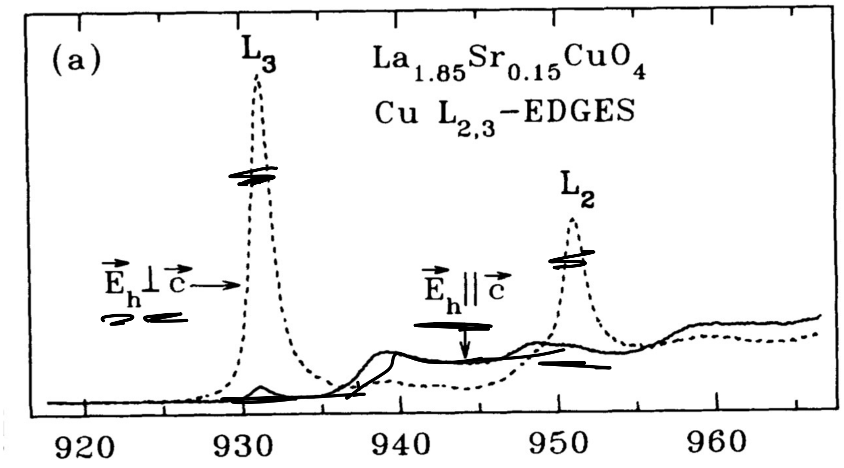
$m = \pm 2$

$$\begin{pmatrix} l' & 1 & l \\ \underset{3d}{\underline{-m'}} & \underline{q} & \underset{2p}{\underline{m}} \end{pmatrix} \qquad |m| \le 1$$

$|m'| = 2$

$\Rightarrow q = \pm 1$ $\quad \vec{E} \parallel (x,y)$ $\quad$ non-zero

$q = 0$ $\quad \vec{E} \parallel z$ $\quad$ zero.



Chen, PRL 68, 2543 (1992)

$$H = \underline{-t\sum_{ij} c^{\dagger}_{i\sigma} c_{j\sigma}} + U\sum_{i} \underline{n_{i\uparrow} n_{i\downarrow}}$$

$$= \underline{H_0} + \underline{H_1}$$

Solve $H_0$:

Hilbert space: $\mathcal{H} \cong \sum_{\sigma} \oint_{T^v} d\vec{k}\, \underline{\underline{\mathcal{H}_{\vec{k}\sigma}}}.$

$\vec{k} \in [0, 2\pi)$

$$H_0 = \begin{array}{cc} |\uparrow\rangle\times(\vec{k}_1, \vec{k}_2, \vec{k}_3 \cdots) & |\downarrow\rangle\times(\vec{k}_1 \cdots \vec{k}_N \\ \left(\begin{matrix} \square & & & 0 \\ & \square & & \\ 0 & & \square & \\ & & & \square \end{matrix}\right. & \left.\begin{matrix} \\ 0 \\ \\ \end{matrix}\right| \\ \hline \left(\begin{matrix} \\ 0 \\ \\ \end{matrix}\right. & \left|\begin{matrix} \square & & & 0 \\ & \square & & \\ & & \square & \\ & & & \ddots \end{matrix}\right) \end{array}$$

$$H_I = \sum \underline{c^{\dagger}_{k+q,\sigma}}\ \underline{c^{\dagger}_{k'-q,\sigma'}}\ \underline{c_{k'\sigma'}}\ \underline{c_{k\sigma}}$$

↳ Some simplification

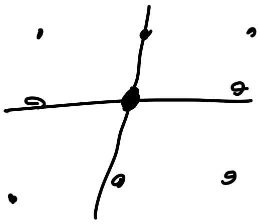
↳ $H = \sum_{k\sigma} \epsilon_k c^{\dagger}_{k\sigma} c_{k\sigma} - V \sum_{k,k',q} c^{\dagger}_{k+q,\uparrow} c^{\dagger}_{-k\downarrow} \underline{c_{-k'+q\downarrow} c_{k'\uparrow}}$

$\underline{\Delta_k} = \underline{V\langle c_{-k\downarrow} c_{k\uparrow}\rangle}$ "$\underline{\text{pairing}}$"

mean-field

$$H_k = \begin{pmatrix} \epsilon_k & -\Delta_k \\ -\bar{\Delta}_k & -\epsilon_k \end{pmatrix} \quad \text{in basis } \{c_{k\uparrow}, c^{\dagger}_{-k\downarrow}\}^T$$

("ODLRO")



$$\Delta_k = \sum_r \underline{\Delta_{\vec r}}\, \underline{e^{i\vec k\cdot\vec r}}$$

expand on near range neighbors.

$$\underline{1}\,,\quad \underbrace{\{\underline{e^{\pm ik_x}},\ \underline{e^{\pm ik_y}}\}}_{NN}.\quad \{\underline{e^{i(k_x\pm k_y)}}.\ \underline{e^{-i(k_x\pm k_y)}}\}$$

construct projectors

$$p^\mu = n_\mu \int_G \overline{\chi^\mu(g)}\, T(g)\, dg$$

for details see Mathematica notebook.

$$P_{A_1} = \frac{1}{4}\begin{pmatrix} 1&1&1&1\\ 1&1&1&1\\ 1&1&1&1\\ 1&1&1&1 \end{pmatrix}$$

(c.f. HW 09. p23)

eigenvector with eigenvalue 1: $\frac{1}{2}(1,1,1,1)^T$

The order parameter in $A_1$ is then

$$e^{ik_x}+e^{ik_y}+e^{-ik_x}+e^{-ik_y} \propto \cos k_x + \cos k_y$$

Similarly. $B_1$ : $\cos k_x - \cos k_y$

$E$ : $[\sin k_x, \sin k_y]$

$A_1$ & $B_1$ even in momentum, ⇒ odd in spin
(singlet pairing)

E odd in momentum ⇒ even in spin
(triplet pairing)

Conventionally denoted as

| | | |
|---|---|---|
| $A_1$ | $B_1$ | E |
| "s" | "d" | "p"-wave superconductivity |

Cuprates are most likely d-wave as shown by e.g. tunneling experiments

Wollman, PRL 71, 2134 (1993)