Recap.

① orbital of l.

$$\chi_l(R) = \underbrace{\sum_{m=-l}^{l} e^{im\theta}}_{\text{proper Rotation}} = \frac{\sin(l+\frac{1}{2})\theta}{\sin\frac{\theta}{2}} \qquad \chi_l(R\otimes i) = (-1)^l \chi_l(R)$$

$$D = V_{l=2} \overset{O_h}{=} E_g \oplus T_{2g} \overset{D_{4h}}{=} (A_{1g}\oplus B_{1g})\oplus(B_{2g}\oplus E_g)$$

$$3z^2-1 \quad x^2-y^2 \quad xy \quad xz/yz$$

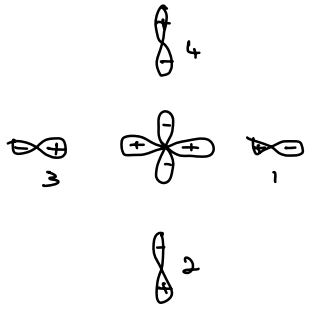
② cuprates: CuO_2 plane as key structure.

Cu: d → E_g ($\uparrow\downarrow$ B_{1g}, $\uparrow$ A_{1g}); T_{2g} ($\uparrow\downarrow$ B_{2g}, $\uparrow\downarrow\uparrow\downarrow$ E_g)

$Cu^{2+} - d^9$ only B_{1g} partially filled.

Oxygens: $V = \text{span}\{p_i^{x,y,z}\}$

For CuO_6 octahedral. dim = 18 one can formally find all irreps. For B_{1g}. one simply considers



$$L_{B_{1g}} = \frac{1}{2}(-p_{1x} - p_{2y} + p_{3x} + p_{4y})$$

$$C_4(z)\cdot L_{B_{1g}} = \frac{1}{2}(-p_{4y} - p_{3x} + p_{2y} + p_{1x})$$

$$= -L_{B_{1g}} \quad \text{etc.}$$

8.6. Dipole selection rules

How do we know that the low-energy model is correct? → using spectroscopy.

In EM field. $\vec{p} \to \vec{p} - q\vec{A} = \vec{p} + e\vec{A}$. The light-matter interaction

$$H_{int} = H_{EM} - H_0 = \frac{(p+eA)^2}{2m} - \frac{p^2}{2m}$$

take the Coulomb gauge $\nabla \cdot A = 0$. then

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

$$= \frac{e}{m}\vec{p}\cdot\vec{A}$$

non-linear term.

small for small $\vec{A}$.

$$\vec{A}(\vec{r}_i) = \frac{1}{\sqrt{V}} \sum_{k,\vec{\epsilon}} \sqrt{\frac{\hbar}{2\omega}} \left(\vec{\epsilon}\, a_{k\vec{\epsilon}}\, e^{i\vec{k}\cdot\vec{r}_i} + h.c. \right)$$

↑ light polarization

Cross section for light absorption: $H = H_e \otimes H_{ph}$.

$$\sigma = \frac{2\pi}{\hbar} \sum |\langle f|H_{int}|i\rangle|^2 \, \delta(E_f - E_i - \omega)$$

$$\langle f|H_{int}|i\rangle \propto e^{ikr} \langle f|\vec{\epsilon}\cdot\vec{p}|i\rangle$$ Dipole approx.

Core electrons. $\propto e^{ikR} \langle f|\vec{\epsilon}\cdot[H, \vec{x}]|i\rangle$

$e^{ikr} \to e^{ikR}$ (↑ elec., ↑ nucleon) $= e^{ikR} \langle f|\vec{\epsilon}\cdot(H\vec{x} - \vec{x}H)|i\rangle$

$= e^{ikR}(E_f - E_i)\langle f|\vec{\epsilon}\cdot\vec{x}|i\rangle$

The dipole operators $D_i = \vec{\epsilon} \cdot \vec{x}_i$

The position in 3D can be expanded by vector operators

$$\vec{x} = x_1 \cdot \hat{e} + x_2 \cdot \hat{e}_2 + x_3 \cdot \hat{e}_3$$

we choose a different basis (irreducible tensor operators)

$$r_q = r\, C_q^{(1)} \qquad q = 0, \pm 1$$

$$C_q^{(1)} = \sqrt{\frac{4\pi}{2k+1}}\, Y_k^q(\hat{r})$$

$$r_{\pm 1} = \mp (x \pm iy)/2 \qquad r_0 = z.$$

Then $\langle f | H_{int} | i \rangle \longrightarrow \langle n'l'm' | r\, C_q^{(1)} | nlm \rangle$

$$= P_{n'l'nl}^{(1)} \langle l'm' | C_q^{(1)} | lm \rangle$$

where $P_{n'l'nl}^{(k)} = \int_0^\infty dr\, r^{k+2} R_{n'l'}(r) R_{nl}(r)$ integral of radial wavefunctions. The remaining matrix element

$$\langle l'm' | C_q^{(k)} | lm \rangle = (-1)^{l'-m'} \begin{pmatrix} l' & k & l \\ -m' & q & m \end{pmatrix} \langle l' \| C^{(k)} \| l \rangle$$

This is the result of Wigner–Eckart theorem.

The first part (Wigner–3J symbol)

$$\begin{pmatrix} l' & k & l \\ -m' & q & m \end{pmatrix} \sim \langle l'm' | k, q; l, m \rangle \quad \text{CG-coefficient}$$

The second part (reduced matrix element) is independent of the magnetic quantum number. only on l's.

$$\langle l' \| C^{(k)} \| l \rangle = (-1)^{l'} \sqrt{(2l+1)(2l'+1)} \begin{pmatrix} l' & k & l \\ 0 & 0 & 0 \end{pmatrix}$$

For the 3J symbol $\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}$ to be nonzero.

it requires

① $|j_i - j_j| \le j_k \le |j_i + j_j|$

② $\sum m_i = 0$

selection rules under this dipole approximation?

$$\begin{pmatrix} l' & k & l \\ -m' & q & m \end{pmatrix} \leftarrow \Delta l = |l - l'| \le k = 1$$

$$\leftarrow \Delta m = m' - m = q \in \{0, \pm 1\}$$

Additionally.

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ -m_1 & -m_2 & -m_3 \end{pmatrix} = (-1)^{j_1+j_2+j_3} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}$$

$\begin{pmatrix} l' & k & l \\ 0 & 0 & 0 \end{pmatrix} \neq 0$ requires $l + l' + 1 = \text{even}$.

$\Delta l \neq 0 \Rightarrow \Delta l = \pm 1$

dipole transition selection rule:

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

Now. to probe Cu-3d related states.

$\Delta l = \pm 1$ requires transitions from/to p or f.
($l=1$) ($l=3$)

It is common to use transition from 2p → 3d.

Consider the x^2-y^2 (B_{1g}) orbital.

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

A. $\begin{pmatrix} l'=2 & q & l=1 \\ -m' & q & m \end{pmatrix}$

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

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

Either from $m=1$ to $m'=2$ via $q=1$

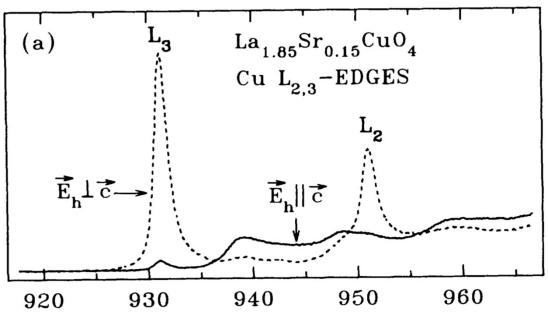
or $m=-1$ to $m'=-2$ via $q=-1$

We know $r_{\pm 1} = \mp (x \pm iy)/2$ $\quad r_0 = z$. which means

$\vec{\epsilon} \,//\, x, y$ can excite p_x / p_y into $d_{x^2-y^2}$

On the other hand. $d_{3z^2-r^2} = Y_{2,0}$

$\vec{\epsilon} \,//\, z$ ($q=0$) can excite p_z ($m=0$) to d_{z^2}.



From another view point:

$\vec{r}$ behaves as $z \rightarrow A_{2u}$ } in D_{4h}.
(as well as p orb) $(x, y) \rightarrow E_u$

z-pol.: $z \otimes P_z = A_{2u} \otimes A_{2u} = A_{1g}$

$z \otimes E_u = A_{2u} \otimes E_u = E_g$

x/y-pol.: $E_u \otimes A_{2u} = E_g$

$E_u \otimes E_u = A_{1g} \oplus A_{2g} \oplus B_{1g} \oplus B_{2g}$

9.7. Superconducting order parameters

Ref: Annett. Advances in Physics. 39. 83 (1990)

Kaba & Sénéchal. PRB 100. 214507 (2019)

use a simplified one-band model. (BCS equation)

$$H = \sum_{k\sigma} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma} + \sum V_{kk'} c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} c_{-k'\downarrow} c_{k'\uparrow}$$

electron-phonon coupling
AFM fluctuations etc.

It is sometimes possible to form "off-diagonal long-range order" (OLRO), or pairing

$$\Delta_k = -\sum_{k'} V_{kk'} \langle c_{-k'\downarrow} c_{k'\uparrow} \rangle$$

Mean-field decoupling: $cc \longrightarrow \langle cc \rangle + (cc - \langle cc \rangle)$

$$H = \sum_{k\sigma} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma} + \sum_{kk'} V_{kk'} c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} c_{-k'\downarrow} c_{k'\uparrow}$$

$$= \sum_{k\sigma} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma} - \sum_k \left(\Delta_k c^\dagger_{k,\uparrow} c^\dagger_{-k\downarrow} + \bar{\Delta}_k c_{-k\downarrow} c_{k\uparrow} \right)$$

$$= \sum_k \left(c^\dagger_{k\uparrow}, c_{-k\downarrow} \right) \begin{pmatrix} \epsilon_k & \bar{\Delta}_k \\ \Delta_k & -\epsilon_{-k} \end{pmatrix} \begin{pmatrix} c_{k\uparrow} \\ c^\dagger_{-k\downarrow} \end{pmatrix} + \text{const.}$$

diagonalized via a Bogoliubov transformation

$$\begin{pmatrix} \gamma_{k\uparrow} \\ \gamma_{-k\downarrow} \end{pmatrix} = \begin{pmatrix} \bar{u}_k & v_k \\ -\bar{v}_k & u_k \end{pmatrix} \begin{pmatrix} c_{k\uparrow} \\ c^{\dagger}_{-k\downarrow} \end{pmatrix}$$

$$\Rightarrow E_k = \sqrt{\epsilon_k^2 + |\Delta_k|^2}$$

We will not discuss more the superconductivity. but the form of Δ_k. In general. we can expand the order parameter as

$$\Delta_k = \sum_i c_i f^i(k)$$

(more generally. $\Delta_{k;mm';\sigma\sigma'} = \sum c_{\alpha\beta\gamma} f^{\alpha}(k) B^{\beta}_{mm'}(k) S^{\gamma}_{\sigma\sigma'}$, for multi-orbital case) (β: band, γ: spin)

We are only discussing one-band singlet pairing.

How to expand? SC has a coherence length. ($\sim$ size of the Cooper pair). we can consider expansions on nearest neighbors.

$$f(k) \to \sum_r f_r \cdot e^{ikr}$$

The Fourier coefficient f_r decays over space.

Consider <u>local</u> pairing $\Delta_k = f_0$ A_{1g}

Consider <u>nearest neighbors</u> $\vec{r} = \hat{x}, \hat{y}$

The four basis function $(e^{ik_x}, e^{-ik_x}, e^{ik_y}, e^{-ik_y})$

Similar to the previous section. we can construct projectors and find eigenstates

$$P_{A_1} = \frac{1}{4}\begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{pmatrix} \qquad 4 = \frac{1}{2}(1, 1, 1, 1)^T$$

The A_1 symmetry is $\frac{1}{2}(e^{ik_x} + e^{ik_y} + e^{-ik_x} + e^{-ik_y})$

$$= \cos k_x + \cos k_y$$

eigen states of P_{B_1}: $\frac{1}{2}(1, -1, 1, -1)^T$

B_1 symmetry: $\frac{1}{2}(\cos k_x - \cos k_y)$

See mathematica notebook for details.

2nd neighbor: $\{e^{i(k_x+k_y)}, e^{i(k_x-k_y)}, e^{-i(k_x+k_y)}, e^{-i(k_x-k_y)}\}$

$V \cong A_1 + B_2 + E$

$A_1 = 2\cos k_x \cos k_y$

$B_2 = 2 \sin k_x \sin k_y$

E: $\sin(k_x + k_y)$

$\sin(k_x - k_y)$

3rd neighbor the same as 1st.

4th neighbor. 8-dim rep. space.

E parity is odd in space → triplet pairing

also → $\sin k_x \pm i \sin k_y$ related by time reversal

gap measurements < transport

ARPES

Josephson tunneling