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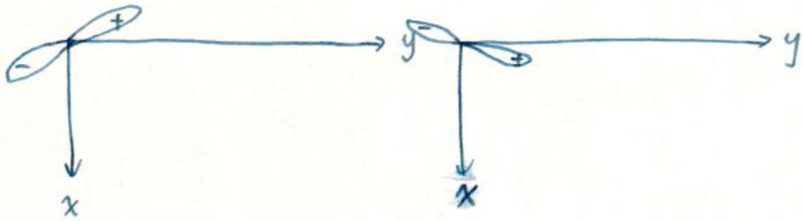
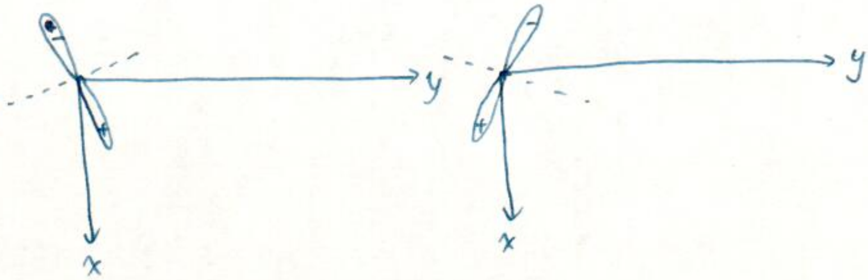
$G_y|d_{yz} A\rangle = -|d_{yz} B\rangle$

$G_y|d_{yz} B\rangle = -|d_{yz} A\rangle$



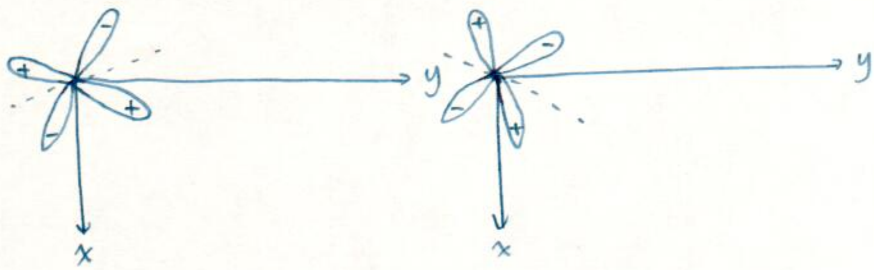
$G_y|d_{zx} A\rangle = |d_{\cancel{\ }zx} B\rangle$

$G_y|d_{zx} B\rangle = |d_{zx} A\rangle$



$G_y|d_{xy} A\rangle = -|d_{xy} B\rangle$

$G_y|d_{xy} B\rangle = -|d_{xy} A\rangle$



$G_y|J_z = \frac{1}{2}, A\ (\underset{x}{\cancel{}}, \underset{y}{\cancel{}}, t)\rangle$

$= \frac{1}{\sqrt{3}}\Big(G_y|d_{yz}\downarrow A\ (x, y, t)\rangle + i\,G_y|d_{zx}\downarrow A\ (x, y, t)\rangle + G_y|d_{xy}\uparrow (x, y, t)\rangle\Big)$

$= \frac{1}{\sqrt{3}}\Big(-|d_{yz}\uparrow B\ (x+\frac{1}{2}, -y+\frac{1}{2}, t)\rangle + i\,|d_{zx}\uparrow B\,(x+\frac{1}{2}, -y+\frac{1}{2}, t)\rangle$

$+ |d_{xy}\downarrow B\ (x+\frac{1}{2}, -y+\frac{1}{2}, t)\rangle\Big)$

$G_y|J_z = \frac{1}{2}, B, (x, y, t)\rangle$

$= \frac{1}{\sqrt{3}}\Big(G_y|d_{yz}\downarrow B\ (x, y, t)\rangle + i\,G_y|d_{zx}\downarrow B\ (x, y, t)\rangle + G_y|d_{xy}\uparrow B\ (x, y, t)\rangle\Big)$

$= \frac{1}{\sqrt{3}}\Big(-|d_{yz}\uparrow A\ (x+\frac{1}{2}, -y+\frac{1}{2}, t)\rangle + i\,|d_{zx}\uparrow A\ (x+\frac{1}{2}, -y+\frac{1}{2}, t)\rangle$

$+ |d_{xy}\downarrow A\,(x+\frac{1}{2}, -y+\frac{1}{2}, t)\rangle\Big)$

$G_y | J_z = -\frac{1}{2}, A\rangle$

$= \frac{1}{\sqrt{3}} \Big(G_y | d_{yz} \uparrow, A, (x, y, t)\rangle - i G_y | d_{zx} \uparrow, A (x, y, t)\rangle$

$- G_y | d_{xy} \downarrow A \ (x, y, t)\rangle \Big)$

$= \frac{1}{\sqrt{3}} \Big(| d_{yz} \downarrow B \ (x+\frac{1}{2}, -y+\frac{1}{2}, t)\rangle + i \ | d_{zx} \downarrow B \ (x+\frac{1}{2}, -y+\frac{1}{2}, t)\rangle$

$+ | d_{xy} \uparrow B \ (x+\frac{1}{2}, -y+\frac{1}{2}, t)\rangle \Big)$

$G_y | J_z = -\frac{1}{2}, B\rangle$

$= \frac{1}{\sqrt{3}} \Big(G_y | d_{yz} \uparrow B \ (x, y, t)\rangle - i G_y | d_{zx} \uparrow, B, (x, y, t)\rangle$

$- G_y | d_{xy} \downarrow B \ (x, y, t)\rangle \Big)$

$= \frac{1}{\sqrt{3}} \Big(| d_{yz} \downarrow A \ (x+\frac{1}{2}, -y+\frac{1}{2}, t)\rangle + i \ | d_{zx} \downarrow, A \ (x+\frac{1}{2}, -y+\frac{1}{2}, t)\rangle$

$+ | d_{xy} \uparrow A (x+\frac{1}{2}, -y+\frac{1}{2}, t)\rangle \Big)$

$\therefore \ G_y | J_z = \frac{1}{2}, A\rangle = - \ | J_z = -\frac{1}{2}, B \ (x+\frac{1}{2}, -y+\frac{1}{2}, t)\rangle$

$G_y | J_z = \frac{1}{2}, B\rangle = - \ | J_z = -\frac{1}{2}, A \ (x+\frac{1}{2}, -y+\frac{1}{2}, t)\rangle$

$G_y | J_z = -\frac{1}{2}, A\rangle = \ | J_z = \frac{1}{2}, B \ (x+\frac{1}{2}, -y+\frac{1}{2}, t)\rangle$

$G_y | J_z = -\frac{1}{2}, B\rangle = \ | J_z = \frac{1}{2}, A, \ (x+\frac{1}{2}, -y+\frac{1}{2}, t)\rangle.$

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Tremblay 논문의 핵심은 nonsymmorphic operator 가 orbital basis 에 apply 되었을 때 basis 가 어떻게 변하는가를 살펴 보는 것이다.

일단 논문을 복습해 보면

$$\phi_{m_\alpha}(\vec{k}) = \frac{1}{\sqrt{N}} \sum_j e^{-i\vec{k}\cdot\vec{R}_j} \phi_{m_\alpha}(\vec{R}_j + \vec{r}_\alpha)$$

이것이 Fourier 변환이고 여기에 nonsymmorphic operator를 취해 보자.

$$\{g|\vec{\tau}\}\phi_{m_\alpha}(\vec{k}) = \frac{1}{\sqrt{N}} e^{-i\vec{k}\cdot\vec{\tau}} \sum_j e^{-i\vec{k}\cdot\vec{R}_j} U_g^{m_\alpha;m'_{\alpha'}} \phi_{m'_{\alpha'}}(g\vec{R}_j + g\vec{r}_\alpha + \vec{\tau})$$

여기서 $e^{-i\vec{k}\cdot\vec{R}_j} = e^{-ig\vec{k}\cdot g\vec{R}_j}$, $g\vec{r}_\alpha + \vec{\tau} = \vec{r}_{\alpha'} + \vec{L}_\alpha$ 로 나타낼수있다.

$$\{g|\vec{\tau}\}\phi_{m_\alpha}(\vec{k}) = \frac{1}{\sqrt{N}} e^{-i\vec{k}\cdot\vec{\tau}} e^{ig\vec{k}\cdot\vec{L}_\alpha} \sum_j e^{-ig\vec{k}\cdot(g\vec{R}_j+\vec{L}_\alpha)} U_g^{m_\alpha;m'_{\alpha'}} \phi_{m'_{\alpha'}}(g\vec{R}_j + \vec{r}_{\alpha'} + \vec{L}_\alpha)$$

$$= e^{-i\vec{k}\cdot\vec{\tau}} e^{ig\vec{k}\cdot\vec{L}_\alpha} U_g^{m_\alpha;m'_{\alpha'}} \phi_{m'_{\alpha'}}(g\vec{k})$$

- - - - - - - -

The action of $\{g|\vec{\tau}\}$ is given by

$$\{g|\vec{\tau}\}\phi_{m_\alpha}(\vec{R}_j + \vec{r}_\alpha) = \phi_{m'_{\alpha'}}(g\vec{R}_j + g\vec{r}_\alpha + \vec{\tau})$$

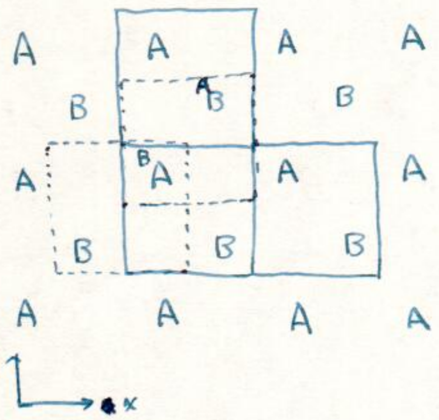
$$= \phi_{m'_{\alpha'}}(g\vec{R}_j + \vec{r}_{\alpha'} + \vec{L}_\alpha)$$

The action of $\{g|\vec{\tau}\}$ on the orbitals ϕ_{m_α} may be represented by a unitary matrix

$$\{g|\vec{\tau}\}\,\phi_{m_\alpha}(\vec{R}_j+\vec{r}_\alpha) = U_g^{m_\alpha;m'_{\alpha'}}\,\phi_{m'_{\alpha'}}(g\vec{R}_j+g\vec{r}_\alpha+\vec{\tau})$$

$$= U_g^{m_\alpha;m'_{\alpha'}}\,\phi_{m'_{\alpha'}}(g\vec{R}_j+\vec{r}_{\alpha'}+\vec{L}_\alpha)$$

그럼 이 원리를 Sr_2IrO_4 에 적용시켜 보자.



$G_x : (x,y,z) \longrightarrow (-x+\frac{1}{2}, y+\frac{1}{2}, t)\times i\sigma_x$

B → A in same unit cell

A → B + $\hat{y}$

$$\phi_{d_{yz},A}(\vec{k}) = \frac{1}{\sqrt{N}}\sum_j e^{-i\vec{k}\cdot\vec{R}_j}\,\phi_{d_{yz},A}(\vec{R}_j+\vec{r}_\alpha)$$

$$G_x\,\phi_{d_{yz},A}(\vec{k}) = \{g|\tfrac{1}{2}\tfrac{1}{2}\}\,\phi_{yz,A}(\vec{k})$$

$$= \frac{1}{\sqrt{N}}e^{-i\vec{k}(\frac{\hat{x}}{2}+\frac{\hat{y}}{2})}\sum_j e^{-i\vec{k}\cdot\vec{R}_j}\,U_g^{d_{yz}A,\,d_{yz}B}\,\phi_{d_{yz}B}(g\vec{R}_j+g\vec{r}_\alpha+\tfrac{\hat{x}}{2}+\tfrac{\hat{y}}{2})$$

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$$= \frac{1}{\sqrt{N}} e^{-i\vec{k}\left(\frac{\hat{x}}{2}+\frac{\hat{y}}{2}\right)} e^{ig\vec{k}\cdot \overset{\vec{L}_\alpha}{\overset{\parallel}{\hat{y}}}} \sum_j e^{-ig\vec{k}\cdot\left(g\vec{R}_j + \overset{\vec{L}_\alpha}{\overset{\parallel}{\hat{y}}}\right)} U_g^{d_{yz}A;d_{yz}B}\, \phi_{d_{yz}B}\left(g\vec{R}_j + \vec{r}_{\alpha'} + \underset{\hat{y}}{\underset{\Downarrow}{\vec{L}_\alpha}}\right)$$

$$= e^{-i\left(\frac{k_x}{2}+\frac{k_y}{2}\right)} e^{ik_y}\, U_g^{d_{yz}A;d_{yz}B}\, \phi_{d_{yz},B}(g\vec{k})$$

한편 G_α 가 $d_{yz}\,B$ orbital 에 apply 하면 $\vec{L}_\alpha = 0$ 이다.

다시말해 다른 unit cell로 가지 않고 같은 unit cell에서 B ~~에서~~ A로

바뀔 뿐이다.

$$\left\{g \,\middle|\, \tfrac{1}{2}\ \tfrac{1}{2}\right\} \phi_{d_{yz}B}(\vec{k})$$

$$= \frac{1}{\sqrt{N}} e^{-i\vec{k}\left(\frac{\hat{x}}{2}+\frac{\hat{y}}{2}\right)} \sum_j e^{-ig\vec{k}\cdot g\vec{R}_j}\, U_g^{d_{yz}B;d_{yz}A}\, \phi_{d_{yz}A}\left(g\vec{R}_j + \vec{r}_{\alpha'}\right)$$

$$= e^{-i\left(\frac{k_x}{2}+\frac{k_y}{2}\right)} U_g^{d_{yz}B;d_{yz}A}\, \phi_{d_{yz}A}(g\vec{k})$$