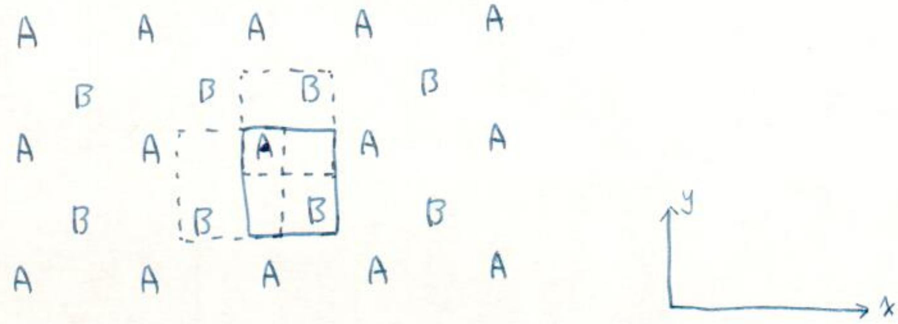
2016 / 10 / 6 (목) (집에서 1)

앞에서는 unit cell dependence 를 보았다면, 여기서는 순수히 nonsymmorphic operator 의 orbital dependence를 보자.

일단 unit cell은 다음과 같이 잡는다.



$B \to A$ same

$A \to B$ $\hat y$

$G_x = \{g|\tfrac{1}{2}\tfrac{1}{2}\}$ $g:(x,y)\to(-x,y)$.

$$\{g|\tfrac{1}{2}\tfrac{1}{2}\}\varphi_{d_{zx}A}(\vec k) = \frac{1}{\sqrt N} e^{-i\vec k(\frac{\hat x}{2}+\frac{\hat y}{2})}\sum_j e^{-i(g\vec k)\cdot(g\vec R_j)} U_g^{d_{zx}A;d_{zx}B}$$

$$\times \varphi_{d_{zx}B}\left(g\vec R_j + g\vec r_\alpha + \frac{\hat x}{2}+\frac{\hat y}{2}\right)$$

$$= \frac{1}{\sqrt N} e^{-i\vec k(\frac{\hat x}{2}+\frac{\hat y}{2})} e^{ig\vec k\cdot(\vec L_\alpha)} \sum_j e^{-ig\vec k(g\vec R_j+\vec L_\alpha)} U_g^{d_{zx}A;d_{zx}B}\varphi_{d_{zx}B}(g\vec R_j + \vec r_{\alpha'}+\vec L_\alpha)$$

$\vec L_\alpha = \hat y$

$$= e^{-i\vec k(\frac{\hat x}{2}+\frac{\hat y}{2})} e^{ik_y} U_g^{d_{zx}A;d_{zx}B}\varphi_{d_{zx}B}(g\vec k).$$

같은 방법으로

$$\{g|\tfrac{1}{2}\tfrac{1}{2}\}\varphi_{d_{zx}B}(\vec k) = e^{-i\vec k(\frac{\hat x}{2}+\frac{\hat y}{2})} U_g^{d_{zx}B;d_{zx}A}\varphi_{d_{zx}A}(g\vec k)$$

$$\{g|\tfrac{1}{2}\tfrac{1}{2}\}\varphi_{d_{xy},A}(\vec k) = e^{-i\vec k(\frac{\hat x}{2}+\frac{\hat y}{2})} e^{ik_y} U_g^{d_{xy}A;d_{xy}B}\varphi_{d_{xy},B}(g\vec k)$$

$$\{g|\tfrac{1}{2}\tfrac{1}{2}\}\varphi_{d_{xy},B}(\vec k) = e^{-i\vec k(\frac{\hat x}{2}+\frac{\hat y}{2})} U_g^{d_{xy}B;d_{xy}A}\varphi_{d_{xy}A}(g\vec k)$$

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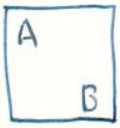
그럼 

이 unit cell 에 대해 $J_{eff} = 1/2$ 상태에 대해서 nonsymmorphic operator 를 적용해 보자.

A → B $\hat{y}$
B → A same unit cell.

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

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

$$= e^{-i\vec{k}\left(\frac{\hat{x}}{2}+\frac{\hat{y}}{2}\right)} e^{ik_y}\, U_g^{J_z=\frac{1}{2}A;\,J_z=-\frac{1}{2}B}\, \varphi_{J_z=-\frac{1}{2},B}(g\vec{k})$$

$$\{g|\tfrac{1}{2}\,\tfrac{1}{2}\}\,\varphi_{J_z=\frac{1}{2}B}(\vec{k}) = e^{-i\vec{k}\cdot\left(\frac{\hat{x}}{2}+\frac{\hat{y}}{2}\right)}\, U_g^{J_z=\frac{1}{2}B;\,J_z=-\frac{1}{2}A}\, \varphi_{J_z=-\frac{1}{2},A}(g\vec{k})$$

$$\{g|\tfrac{1}{2}\,\tfrac{1}{2}\}\,\varphi_{J_z=-\frac{1}{2},A}(\vec{k}) = e^{-i\vec{k}\cdot\left(\frac{\hat{x}}{2}+\frac{\hat{y}}{2}\right)} e^{ik_y}\, U_g^{J_z=-\frac{1}{2}A;\,J_z=\frac{1}{2}B}\, \varphi_{J_z=\frac{1}{2},B}(g\vec{k})$$

$$\{g|\tfrac{1}{2}\,\tfrac{1}{2}\}\,\varphi_{J_z=-\frac{1}{2},B}(\vec{k}) = e^{-i\vec{k}\cdot\left(\frac{\hat{x}}{2}+\frac{\hat{y}}{2}\right)}\, U_g^{J_z=-\frac{1}{2}B;\,J_z=\frac{1}{2}A}\, \varphi_{J_z=\frac{1}{2},A}(g\vec{k})$$

$$\{g|\tfrac{1}{2}\,\tfrac{1}{2}\}\begin{pmatrix}\varphi_{J_z=\frac{1}{2}A}(\vec{k})\\ \varphi_{J_z=\frac{1}{2}B}(\vec{k})\\ \varphi_{J_z=-\frac{1}{2}A}(\vec{k})\\ \varphi_{J_z=-\frac{1}{2}B}(\vec{k})\end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & i e^{-i\vec{k}\left(\frac{\hat{x}}{2}+\frac{\hat{y}}{2}\right)} e^{ik_y} \\ 0 & 0 & i e^{-i\vec{k}\cdot\left(\frac{\hat{x}}{2}+\frac{\hat{y}}{2}\right)} & 0 \\ 0 & i e^{-i\vec{k}\left(\frac{\hat{x}}{2}+\frac{\hat{y}}{2}\right)} e^{ik_y} & 0 & 0 \\ i e^{-i\vec{k}\cdot\left(\frac{\hat{x}}{2}+\frac{\hat{y}}{2}\right)} & 0 & 0 & 0 \end{pmatrix}\begin{pmatrix}\phi_{\frac{1}{2}A}\\ \phi_{\frac{1}{2}B}\\ \phi_{-\frac{1}{2}A}\\ \phi_{-\frac{1}{2}B}\end{pmatrix}$$

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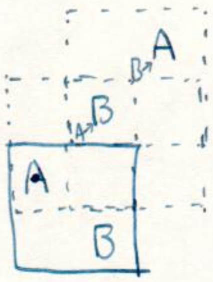
$$= e^{-i\vec{k}\left(\frac{\hat{x}}{2}+\frac{\hat{y}}{2}\right)} \begin{pmatrix} e^{ik_y} & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & e^{ik_y} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & 0 & 0 & i \\ 0 & 0 & i & 0 \\ 0 & i & 0 & 0 \\ i & 0 & 0 & 0 \end{pmatrix}$$

그럼 $G_y = \{\sigma_y | \frac{1}{2}\ \frac{1}{2}\}$ 는 어떨까? $\sigma_y : (x, y) \to (x, -y)$

$$\{\sigma_y | \tfrac{1}{2}\ \tfrac{1}{2}\} \varphi_{J_z=\frac{1}{2}, A}(\vec{k}) = \frac{e^{-i\vec{k}\left(\frac{\hat{x}}{2}+\frac{\hat{y}}{2}\right)}}{\sqrt{N}} e^{i(g\vec{k})\cdot\vec{L}_\alpha} \sum_j e^{-i(g\vec{k})\cdot(g\vec{R}_j + \vec{L}_\alpha)} U_g^{J_z=\frac{1}{2}A;\, J_z=-\frac{1}{2}B} \varphi_{J_z=-\frac{1}{2}B}(g\vec{R}_j + \vec{r}_{\alpha'} + \vec{L}_\alpha)$$



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

$A \to B \quad \hat{y}$

$B \to A \quad \hat{x}+\hat{y}$.

$$= e^{-i\vec{k}\cdot\left(\frac{\hat{x}}{2}+\frac{\hat{y}}{2}\right)} e^{-ik_y} U_g^{J_z=\frac{1}{2}A;\, J_z=-\frac{1}{2}B} \varphi_{J_z=-\frac{1}{2}B}(g\vec{k}).$$

$$\{\sigma_y | \tfrac{1}{2}\ \tfrac{1}{2}\} \varphi_{J_z=\frac{1}{2}B}(\vec{k}) = e^{-i\vec{k}\cdot\left(\frac{\hat{x}}{2}+\frac{\hat{y}}{2}\right)} e^{i(k_x-k_y)} U_g^{J_z=\frac{1}{2}A;\, J_z=-\frac{1}{2}B} \varphi_{J_z=-\frac{1}{2}B}(g\vec{k})$$

$$\{\sigma_y | \tfrac{1}{2}\ \tfrac{1}{2}\} \varphi_{J_z=-\frac{1}{2}A}(\vec{k}) = e^{-i\vec{k}\cdot\left(\frac{\hat{x}}{2}+\frac{\hat{y}}{2}\right)} e^{-ik_y} U_g^{J_z=-\frac{1}{2}A;\, J_z=\frac{1}{2}B} \varphi_{J_z=\frac{1}{2}B}(g\vec{k})$$

$$\{\sigma_y | \tfrac{1}{2}\ \tfrac{1}{2}\} \varphi_{J_z=-\frac{1}{2}B}(\vec{k}) = e^{-i\vec{k}\cdot\left(\frac{\hat{x}}{2}+\frac{\hat{y}}{2}\right)} e^{i(k_x-k_y)} U_g^{J_z=-\frac{1}{2}B;\, J_z=\frac{1}{2}A} \varphi_{J_z=\frac{1}{2}A}(g\vec{k}).$$

2016 / 10 / 6 (목) (집에서 4)

$$\{\sigma_y | \tfrac{1}{2}\ \tfrac{1}{2}\} \begin{pmatrix} \varphi_{J_z=\frac{1}{2}A}(\vec{k}) \\ \varphi_{J_z=\frac{1}{2}B}(\vec{k}) \\ \varphi_{J_z=-\frac{1}{2}A}(\vec{k}) \\ \varphi_{J_z=-\frac{1}{2}B}(\vec{k}) \end{pmatrix} = e^{-i\left(\frac{k_x}{2}+\frac{k_y}{2}\right)} \begin{pmatrix} 0 & 0 & 0 & -e^{-ik_y} \\ 0 & 0 & -e^{i(k_x-k_y)} & 0 \\ 0 & e^{-ik_y} & 0 & 0 \\ e^{i(k_x-k_y)} & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \phi_{J_z=\frac{1}{2}A}(g\vec{k}) \\ \phi_{J_z=\frac{1}{2}B}(g\vec{k}) \\ \phi_{J_z=-\frac{1}{2}A}(g\vec{k}) \\ \phi_{J_z=-\frac{1}{2}B}(g\vec{k}) \end{pmatrix}$$

$$\begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} e^{ik_y} & 0 & 0 & 0 \\ 0 & e^{-i(k_x-k_y)} & 0 & 0 \\ 0 & 0 & e^{ik_y} & 0 \\ 0 & 0 & 0 & e^{-i(k_x-k_y)} \end{pmatrix} \cdot H_k \cdot$$

$$\begin{pmatrix} e^{-ik_y} & 0 & 0 & 0 \\ 0 & e^{i(k_x-k_y)} & 0 & 0 \\ 0 & 0 & e^{-ik_y} & 0 \\ 0 & 0 & 0 & e^{i(k_x-k_y)} \end{pmatrix} \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}$$

$$= \begin{pmatrix} \varepsilon_{00}(\vec{k},\theta) & e^{-ik_x}\left(\varepsilon_{0x}(\vec{k},\theta) - i\,\varepsilon_{zy}(\vec{k},\theta)\right) & 0 & 0 \\ e^{ik_x}\left(\varepsilon_{0x}(\vec{k},\theta) + i\,\varepsilon_{zy}(\vec{k},\theta)\right) & \varepsilon_{00}(\vec{k},\theta) & 0 & 0 \\ 0 & 0 & \varepsilon_{00}(\vec{k},\theta) & e^{-ik_x}\left(\varepsilon_{0x}(\vec{k},\theta) + i\,\varepsilon_{zy}(\vec{k},\theta)\right) \\ 0 & 0 & e^{ik_x}\left(\varepsilon_{0x}(\vec{k},\theta) - i\,\varepsilon_{zy}(\vec{k},\theta)\right) & \varepsilon_{00}(\vec{k},\theta) \end{pmatrix}$$