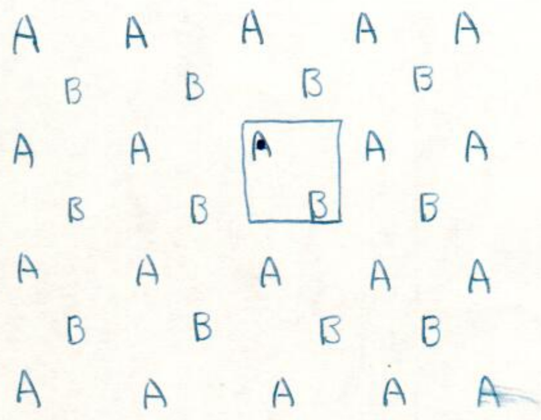
2016/10/6 (목) (1)

- 논의는 nonsymmorphic operator를 orbital basis에 적용시키면 sublattice에 따라서 extra phase가 다르게 나타난다는 것이다.

그럼 문제는 unit cell을 어떻게 잡느냐가 관건일 수도 있겠다.

우리가 다루는 Sr_2IrO_4 system의 경우



먼저 inversion center를 정하자.

unit cell을 잡는데 4가지 경우가 있을 수 있다.

4가지 경우에 따라서 extra phase가 다른데

unitary transform을 하고 나면 두가지 경우만 남는다.

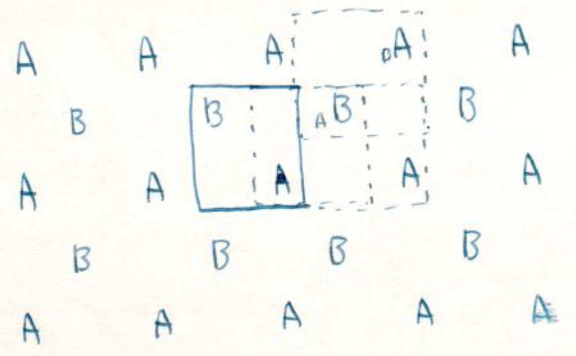
$$\begin{pmatrix} \varepsilon_{00}(\vec{k},\theta) & e^{ik_y}(\varepsilon_{0x}(\vec{k},\theta)-i\varepsilon_{zy}(\vec{k},\theta)) & 0 & 0 \\ e^{-ik_y}(\varepsilon_{0x}(\vec{k},\theta)+i\varepsilon_{zy}(\vec{k},\theta)) & \varepsilon_{00}(\vec{k},\theta) & 0 & 0 \\ 0 & 0 & \varepsilon_{00}(\vec{k},\theta)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

와

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

2016/10/6 (목) (2)

구체적으로 unitary matrix 구하는 방법은



$B \rightarrow A \quad \hat{x}+\hat{y} = \vec{L}_x$

$A \rightarrow B \quad \hat{x} = \vec{L}_x$

$G_x = \{ g \mid \tfrac{1}{2}\ \tfrac{1}{2} \} \qquad g : (x,y) \rightarrow (-x,y)$

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

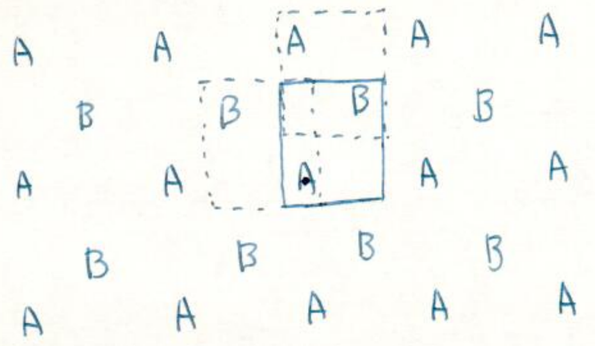
$$\{g|\tfrac{1}{2}\tfrac{1}{2}\}\varphi_{J_z=\frac{1}{2},B}(\vec{k}) = e^{-i\vec{k}\cdot\left(\frac{\hat{x}}{2}+\frac{\hat{y}}{2}\right)} e^{i(g\vec{k})\cdot(\hat{x}+\hat{y})} U_g^{J_z=\frac{1}{2}B\,;\,J_z=-\frac{1}{2}A} \varphi_{J_z=-\frac{1}{2}A}(g\vec{k})$$

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

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

$$\therefore\ e^{-i\left(\frac{k_x}{2}+\frac{k_y}{2}\right)} \begin{pmatrix} e^{-ik_x} & 0 & 0 & 0 \\ 0 & e^{-i(k_x-k_y)} & 0 & 0 \\ 0 & 0 & e^{-ik_x} & 0 \\ 0 & 0 & 0 & e^{-i(k_x-k_y)} \end{pmatrix} \begin{pmatrix} 0 & 0 & 0 & i \\ 0 & 0 & i & 0 \\ 0 & i & 0 & 0 \\ i & 0 & 0 & 0 \end{pmatrix}$$

다른 unit cell 의 예.



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

$A \to B \quad$ same.

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

$= G_x \quad g:(x,y)\to(-x,y)$

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

$$\{g|\tfrac{1}{2}\,\tfrac{1}{2}\}\,\varphi_{J_z=-\frac{1}{2}A}(\vec{k}) = e^{-i\left(\frac{k_x}{2}+\frac{k_y}{2}\right)}\, e^{i\cdot 0}\, U_g^{J_z=-\frac{1}{2}A\,;\,J_z=\frac{1}{2}B}\,\varphi_{J_z=\frac{1}{2}B}(g\vec{k})$$

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

$$\therefore\; e^{-i\left(\frac{k_x}{2}+\frac{k_y}{2}\right)}\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & e^{ik_y} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & e^{ik_y}\end{pmatrix}\begin{pmatrix} 0 & 0 & 0 & i \\ 0 & 0 & i & 0 \\ 0 & i & 0 & 0 \\ i & 0 & 0 & 0\end{pmatrix}.$$