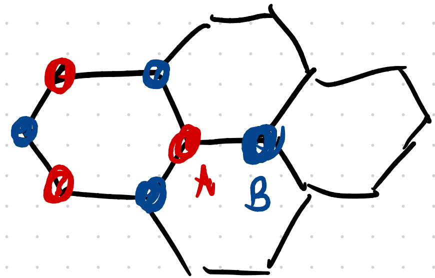
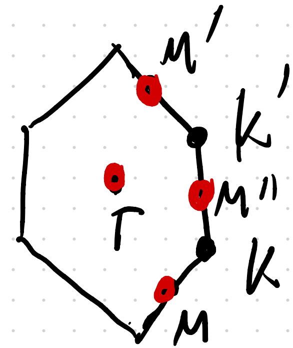
Lecture 25

Recap: Kane-Mele model

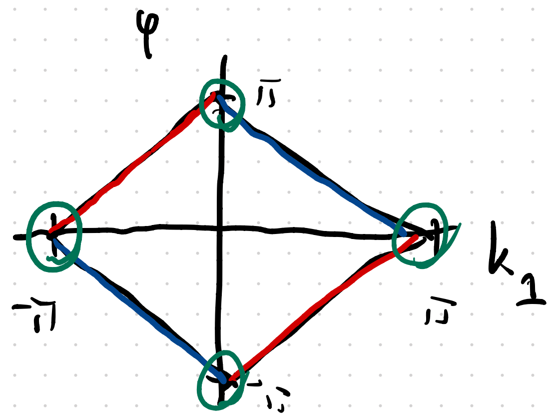


BZ



With S.O.C

degeneracies protected by TRS (Kramers theorem)



$\nu = 1$

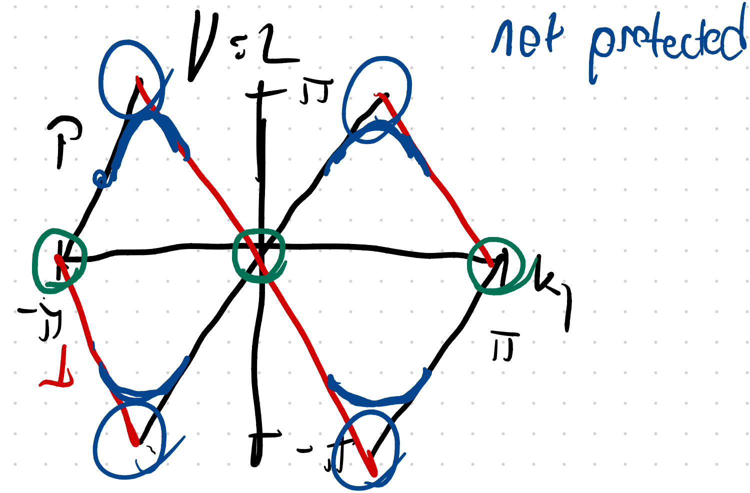
ν - helical winding number

$\nu = \{0, 1\}$ - $\mathbb{Z}_2$ invariant

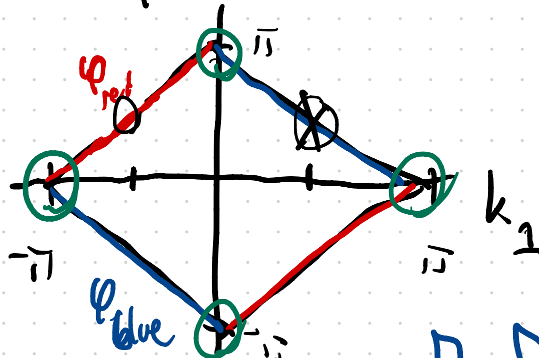
"Kane-Mele invariant"

Chern # for Kane-Mele model = 0

protected by TRS



$\mathbb{Z}_2$ invariants and Wannier Functions



$\nu = 1$

$$P_{x_2} P |W_{red\,R_2 k_1}\rangle = \left(R_2 + \frac{\varphi_{red}(k_1)}{2\pi}\right) |W_{red\,R_2 k_1}\rangle$$

$$P_{x_2} P |W_{blue\,R_2 k_1}\rangle = \left(R_2 + \frac{\varphi_{blue}(k_1)}{2\pi}\right) |W_{blue\,R_2 k_1}\rangle$$

$$U_T |W_{red\,R_2 k_1}\rangle = |W_{blue\,R_2 -k_1}\rangle$$

$$U_T |W_{blue\,R_2, +k_1}\rangle = -|W_{red\,R_2 k_1}\rangle$$

Lets look for Wannier functions

$|W_{red\,\vec{R}}\rangle$ $|W_{blue\,\vec{R}}\rangle$ that satisfy the properties

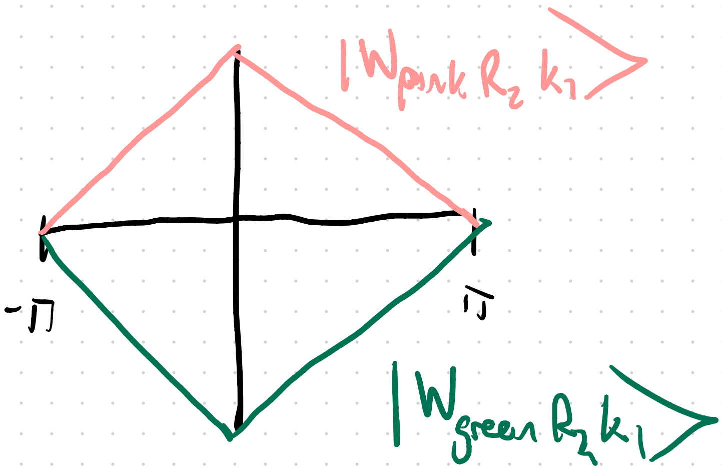
true for isolated atoms

① Both exponentially localized

② $U_T |W_{red\,\vec{R}}\rangle = |W_{blue\,\vec{R}}\rangle$

$U_T |W_{blue\,\vec{R}}\rangle = -|W_{red\,\vec{R}}\rangle$

$\nu = 1 \Rightarrow$ Wannier functions satisfying 1 and 2 don't exist!



$\mathbb{Z}_2$ invariant is an obstruction to finding Wannier fns that are <u>both</u> exponentially localized & Time-reversal symmetric

$\boxed{\text{Soluyanov Vanderbilt 2011}}$

Topological Crystalline insulators: an insulator whose occupied bands do not allow for exponentially localized Wannier functions that respect the crystal symmetries

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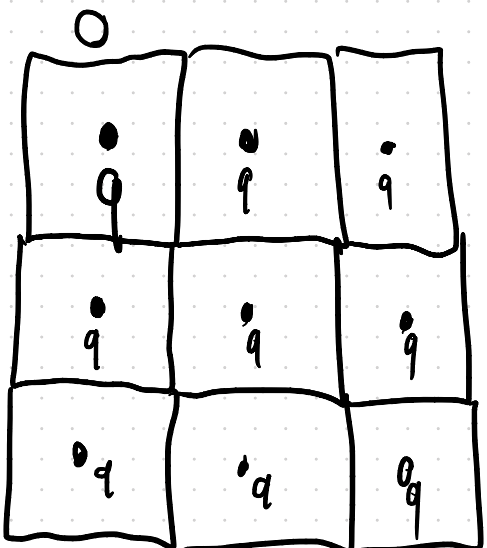
Topological Quantum Chemistry / Symmetry-based indicators of band topology

Outline: - Define symmetric, exponentially localized Wannier functions in terms of space group reps

- Collect symmetry data (irreps of the little grp) for trivial bands
- Define indicators for nontrivial bands in terms of symmetry data



translation symmetry: identical atom at $\vec{q}+\vec{R}$ for all Bravais lattice vectors $\vec{R}$

Valence orbitals $|W_{n\vec{R}}\rangle$

n ← orbital index, $\vec{R}$ ← unit cell index

$$|W_{n\vec{R}}\rangle = U_{\vec{R}} |W_{n0}\rangle$$

Other symmetries in the space group G:

site-symmetry group $G_{\vec{q}} \subset G$

$$G_{\vec{q}} = \{ g \in G \mid g\vec{q} = \vec{q} \}$$

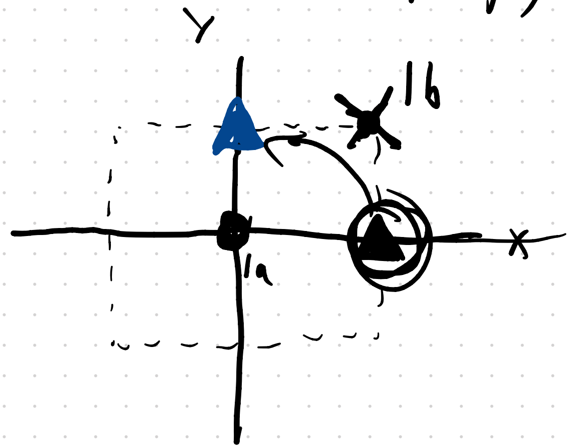
if $|W_{n\vec{0}}\rangle$ are centered at $\vec{q}$, then they must transform in some representation of G_q

$$U_{g_q}|W_{n\vec{0}}\rangle = |W_{m0}\rangle \rho_{mn}(g_q)$$

ρ_i is a representation of the site symmetry group

Example: $p4mm \quad \langle a\hat{x}, a\hat{y}, C_{4z}, M_x \rangle$

Wyckoff positions



$1a \; (0,0)$: $G_{1a} = \langle C_{4z}, M_x \rangle \cong 4mm$

$1b$: $\left(\frac{a}{2}, \frac{a}{2}\right) \quad G_{1b} = \langle \{C_{4z} | a\hat{x}\}, \{M_x | a\hat{y}\} \rangle \cong 4mm$

$2c$: $\left(\frac{a}{2}, 0\right) \quad G_{2c} = \langle M_x, \{C_{2z} | a\hat{x}\} \rangle$

$$\cong 2mn$$

$$\left(0, \frac{q}{2}\right) = C_{4z}\left(\frac{q}{2}, 0\right)$$

$$G_{\left(0,\frac{q}{2}\right)} = C_{4z}\, G_{\left(\frac{q}{2},0\right)}\, C_{4z}^{-1}$$

$$G_{\vec{q}} \cup \vec{e}_1 G_{\vec{q}} \cup \vec{e}_2 G_{q} \cdots \quad TG_{\vec{q}}$$

we know how every element of $TG_{\vec{q}}$ acts on $|W_{n\vec{R}}\rangle$

$$|W_{nR}\rangle = U_{\vec{R}}|W_{n0}\rangle \qquad \vec{t}\, g_{\vec{q}}$$

$$g_{\vec{q}} = \{\bar{g}|\vec{d}\}$$

$$U_{t g_{\vec{q}}}|W_{nR}\rangle = U_{\vec{t}}\, U_{g_{\vec{q}}}\, U_{\vec{R}}|W_{n0}\rangle$$

$$g_q \vec{R} = \{\bar{g}|\vec{d} + \bar{g}\vec{R}\} = \{E|\bar{g}\vec{R}\}\, g_{\vec{q}}$$

$$= U_{\bar{g}\vec{R}+\vec{t}}\, U_{g_q}|W_{n0}\rangle$$

$$= U_{\bar{g}R+t} |W_{m0}\rangle \rho_{mn}(g_q)$$

$$= |W_{m\,\bar{g}R+t}\rangle \rho_{mn}(g_q)$$

$|W_{n\vec{R}}\rangle$ give us a representation of $TG_{\vec{q}}$