Lecture 18

Last lecture: $|W_{aR}\rangle$ - exponentially localized Wannier functions

tight-binding basis functions $|\chi_{ak}\rangle = \sum_R e^{i\vec{k}\cdot(R+\langle r_a\rangle)} |W_{aR}\rangle$

$$|\psi_{nk}\rangle = \sum_a u^a_{nk} |\chi_{ak}\rangle$$

$$\sum_b h^{ab}(k) u^b_{nk} = E_{nk} u^a_{nk}$$

tight-binding Bloch Hamiltonian

$$h^{ab}(k) = \sum_R \langle W_{aR}|H|W_{bR'}\rangle e^{-ik(R-R'+\langle r_a\rangle - \langle r_b\rangle)}$$

We can truncate $\langle W_{aR}|H|W_{bR'}\rangle$ to some short range if $|W_{aR}\rangle$ are exponentially localized

Symmetries: Suppose H is invariant under a space group G

We want $\{|W_{aR}\rangle\}$ to transform in a representation of G

Band representation $\qquad W_{aR}(r) = \langle r|W_{aR}\rangle$

① $W_{aR}(r)$ is centered at $\langle r_a\rangle + R$

$$W_{aR}(r) = W_a(r - R - \langle r_a\rangle)$$

$\langle r|U_{\{E|\vec{t}\}}|W_{aR}\rangle$

$= \langle r-\vec{t}\,|W_{aR}\rangle$

$= W_{aR}(r-\vec{t})$

$= W_a(r-R-t-\langle r_a\rangle)$

$= W_{aR+t}(r)$

$\rightsquigarrow \quad U_{\{E|\vec{t}\}}|W_{aR}\rangle = |W_{aR+\vec{t}}\rangle$

Wannier functions transform in a (infinite dimensional) representation of the Bravais lattice

② $g = \{\bar{g} | \delta\} \in G$

always true

$$\boxed{\begin{aligned} \langle r | U_g | W_{aR} \rangle &= W_{aR}(g^{-1}\vec{r}) \\ &= W_{aR}(\bar{g}^{-1}\vec{r} - \bar{g}^{-1}\delta) \\ &= W_a(g^{-1}(\vec{r} - g(R + \langle r_a \rangle))) \end{aligned}}$$

$\Rightarrow$ we want

$$= \sum_b W_b(r - R' - \langle r_b \rangle) B_{ba}(g)$$

— need $R' = g(R + \langle r_a \rangle) - \langle r_b \rangle$

$$\boxed{U_g | W_{aR} \rangle = \sum_b | W_{bR'} \rangle B_{ba}(g) \, \delta_{R', g(R + \langle r_a \rangle) - \langle r_b \rangle}}$$

$B_{ba}(g)$ form a representation of the space group

$B_{ba}(\{E|\vec{t}\}) = \delta_{ab}$ $\Rightarrow$ $B_{ab}(g)$ give a representation of G_{Γ} - determined by point group representations

$$B_{ba}(g) = B_{ba}(\bar{g})$$ only depends on the point group

How do symmetries act on tight-binding basis fns:

$$U_{\{\bar{g}|\delta\}} |\chi_{ak}\rangle = \sum_R U_{\{\bar{g}|\delta\}} |W_{aR}\rangle e^{ik\cdot(R+\langle r_a\rangle)}$$

$$= \sum_{R R' b} |W_{bR'}\rangle B_{ba}(\bar{g})\, \delta_{R',\, g(R+\langle r_a\rangle)-\langle r_b\rangle}\, e^{ik\cdot(R+\langle r_a\rangle)}$$

$$g(R+\langle r_a\rangle)-\langle r_b\rangle$$

$$= \bar{g}(R+\langle r_a\rangle)+\vec{\delta}-\langle r_b\rangle$$

$$R = \bar{g}^{-1}(R'+\langle r_b\rangle-\vec{\delta})-\langle r_a\rangle$$

$$\vec{k}\cdot\vec{x} = (\bar{g}k)\cdot(\bar{g}x)$$

$$= \sum_{R' b} |W_{bR'}\rangle B_{ba}(\bar{g})\, e^{ik\cdot(\bar{g}^{-1}(R'+\langle r_b\rangle-\vec{\delta}))}$$

$$= \sum_{R' b} |W_{bR'}\rangle e^{i\bar{g}k\cdot(R'+\langle r_b\rangle)} B_{ba}(\bar{g})\, e^{-i\bar{g}k\cdot\vec{\delta}}$$

$$= \sum_{b} |\chi_{b\bar{g}k}\rangle \left[B_{ba}(\bar{g})\, e^{-i\bar{g}k\cdot\vec{\delta}}\right]$$

$$\boxed{U_{\{\bar{g}|\vec{\delta}\}} |\chi_{ak}\rangle = \sum_{b} |\chi_{b\bar{g}k}\rangle \left[B_{ba}(\bar{g})\, e^{-i\bar{g}k\cdot\vec{\delta}}\right]}$$

$$h^{ab}(k) = \sum_{R} \langle W_{aR}|H|W_{bR'}\rangle e^{-ik(R-R'+\langle r_a\rangle-\langle r_b\rangle)}$$

$$= \langle \chi_{ak}|H|\chi_{bk}\rangle$$

H invariant under space group $G \Rightarrow \ [U_g, H]=0 \ \forall g\in G$

$$\Rightarrow \quad h^{ab}(k) = \left(\langle \chi_{ak}|U_g^{\dagger}\right) H \left(U_g|\chi_{bk}\rangle\right)$$

$$= \sum_{cd} \cancel{e^{i\bar{g}k\cdot\vec{s}}}\, B^{\dagger}_{ac}(\bar{g})\langle \chi_{c\bar{g}k}|H|\chi_{d\bar{g}k}\rangle B_{da}(\bar{g})\cancel{e^{-i\bar{g}k\cdot\vec{s}}}$$

$$\boxed{h(k) = B^{\dagger}(\bar{g})\, h(\bar{g}k)\, B(\bar{g}) \quad \text{for all } \{\bar{g}|\vec{\delta}\} \in G}$$

(This relation holds for truncated (ie. Nearest Neighbor) Hamiltonians as well, as long as we truncate in a symmetric way)

$$|\chi_{ak}\rangle = \sum_R |W_{aR}\rangle e^{ik\cdot(R+\langle r_a\rangle)}$$

$\vec{b} \in$ reciprocal lattice

$$|\chi_{a\vec{k}+\vec{b}}\rangle = \sum_R |W_{aR}\rangle e^{i(\vec{k}+\vec{b})\cdot(R+\langle r_a\rangle)}$$

$$= \sum_R |W_{aR}\rangle e^{i\vec{k}\cdot(R+\langle r_a\rangle)}\, e^{i\vec{b}\cdot\langle r_a\rangle}$$

$$= |\chi_{ak}\rangle e^{i\vec{b}\cdot\langle r_a\rangle}$$

eigenfunctions $\quad |\psi_{nk+\vec{b}}\rangle = |\psi_{nk}\rangle = \sum_a u^a_{nk} |\chi_{ak}\rangle$

$$u^a_{nk+\vec{b}} = u^a_{nk} e^{-i\vec{b}\cdot\langle r_a\rangle}$$

Introduce $V_{ab}(\vec{b}) = e^{i\vec{b}\cdot\langle r_a\rangle}\delta_{ab}$

$$\vec{u}_{n\vec{k}+\vec{b}} = V^\dagger(b)\vec{u}_{nk}$$

$$h(k+\vec{b}) = V^\dagger(b)\, h(k)\, V(b)$$

if we focus on $\vec{k}_*$ and $G_{k_*} \ni g$

$$h(k_*) = B^\dagger(\bar{g})\, h(\vec{k}_* + \vec{b}_g)\, B(\bar{g}) \qquad g\vec{k}_* = \vec{k}_* + \vec{b}_g$$

$$= B^\dagger(\bar{g}) V^\dagger(b_g) h(k_*) V(b_g) B(\bar{g})$$

$$\Rightarrow \left[V(b_g) B(\bar{g}) e^{-i\bar{g}k\cdot\vec{\delta}}, h(k_*) \right] = 0$$

$\left\{ V(\vec{b}_g) B(\bar{g}) e^{-i\bar{g}k\cdot\vec{\delta}} \right\}$ form a representation of G_{k*}

Berry connection in the tight-binding basis:

$$|\psi_{nk}\rangle = \sum_a u^a_{nk} |\chi_{ak}\rangle$$

$$u_{nk}(r) = e^{-ik\cdot r}\psi_{nk}(r) = \sum_{a} u^{a}_{nk} e^{-ik\cdot r}\chi_{ak}(r)$$

$$= \sum_{aR} u^{a}_{nk}\, W_{aR}(r)\, e^{ik\cdot(R+\langle r_a\rangle - r)}$$

Lets evaluate $A^{nm}_{\mu}(k) = i\left\langle u_{nk} \middle| \frac{\partial u_{mk}}{\partial k_\mu}\right\rangle_{cell}$

$$A^{nm}_{\mu}(k) = i\int_{cell} d^3y\, u_{nk}(y)\frac{\partial u_{mk}(y)}{\partial k_\mu}$$

$$= i\int_{cell} d^3y \sum_{aR}\sum_{bR'} \left(u^{a}_{nk}\right)^{*} e^{-ik\cdot(R+\langle r_a\rangle - y)}\, W^{*}_{aR}(y)\,\frac{\partial}{\partial k_\mu}\left[u^{b}_{mk} W_{bR'}(y)\, e^{ik\cdot(R'+\langle r_b\rangle - y)}\right]$$

$$= i\int_{\text{cell}} d^3y \sum_{aR\,bR'} e^{ik\cdot(R'+\langle r_b\rangle - R - \langle r_a\rangle)} W^{\dagger}_{aR}(y) W_{bR'}(y) \left[\underbrace{(u^a_{nk})^{\dagger} \frac{\partial u^b_{mk}}{\partial k_\mu}}_{1} + \underbrace{i\, u^{a\dagger}_{nk} u^b_{mk} (R' + \langle r_b\rangle - y)}_{2} \right]$$

$$1 \quad i\int_{\text{cell}} d^3y\, \chi^{\dagger}_{ak}(y)\chi_{bk}(y) (u^a_{nk})^{\dagger} \frac{\partial u^b_{mk}}{\partial k_\mu} = i\, \vec{u}^{\,\dagger}_{nk} \cdot \frac{\partial}{\partial k_\mu} \vec{u}_{mk}$$

Berry connection of the tight-binding eigenvectors $\vec{u}_{nk}$

" tight-binding Berry connection

2 Always true: $\langle W_{aR} | W_{bR'} \rangle = \delta_{RR'}\delta_{ab}$

Useful approximation: $\langle W_{aR} | \vec{x} | W_{bR'} \rangle = \delta_{ab} \delta_{RR'} (R + \langle r_a \rangle)$

strict tight-binding limit

(2) vanishes in this approximation

$$A_\mu^{nm}(k) \longrightarrow i \vec{u}_{nk}^{\dagger} \cdot \frac{\partial u_{mk}}{\partial k_\mu}$$

If $\langle W_{aR} | \vec{x} | W_{bR'} \rangle$ is diagonal, $h(k)$, E_{nk}, $A_\mu(k)$ only depend on the centers of the Wannier fns