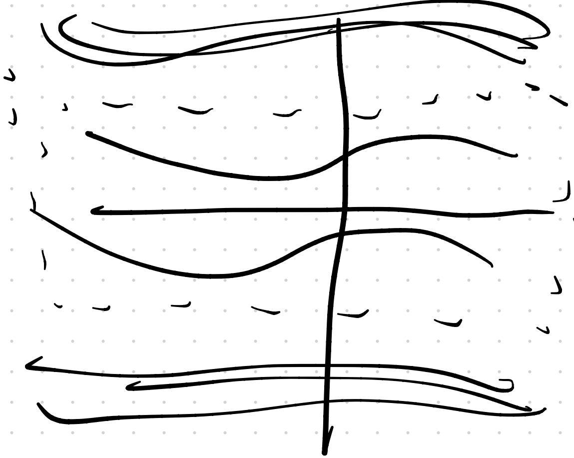
Lecture 19

Recap:



Wannier functions $|w_{a\vec{R}}\rangle$

are centered at $\vec{R} + \bar{r}_a$

tight-binding basis functions $|\chi_{a\vec{k}}\rangle = \sum_R e^{ik\cdot(R+\bar{r}_a)} |w_{aR}\rangle$

tight-binding hamiltonian $h^{ab}(k) = \langle \chi_{a\vec{k}} | H | \chi_{bk} \rangle$

we can truncate this to obtain approximations

(approximate) energy eigenstates

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

finite-dimensional matrix eqn.

operator eqn $\rightarrow$ $$H|\psi_{nk}\rangle = E_{nk}|\psi_{nk}\rangle \iff \boxed{h(k)\vec{u}_{nk} = E_{nk}\vec{u}_{nk}}$$

$$|\chi_{a\vec{k}+\vec{G}}\rangle = V(\vec{G})|\chi_{a\vec{k}}\rangle \qquad \vec{G} \in \check{T}$$ reciprocal lattice vector

$$V_{ab}(G) = e^{i\vec{G}\cdot\vec{r}_a}\delta_{ab}$$

$$\vec{u}_{nk+G} = V^\dagger(\vec{G})\vec{u}_{nk}$$

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

In some cases, if H is invariant under the symmetries of a space group $\vec{G}$, then we can look for $|W_{a\vec{R}}\rangle$ transforming in a <u>band representation</u>

$$g = \{\bar{g}|\vec{d}\} \in G \qquad u_g|W_{a\vec{R}}\rangle = \sum_b |W_{b,\,g(R+\bar{r}_a)-\bar{r}_b}\rangle B_{ba}(\bar{g})$$

$B_{ba}(\bar{g})$: representation of the point group $\bar{G} = G/T$

$$u_g|\chi_{a\vec{k}}\rangle = \sum_b |\chi_{b\,\bar{g}k}\rangle B_{ba}(\bar{g})\, e^{-i\bar{g}k\cdot\vec{d}}$$

$$h(k) = B^{+}(\bar{g})\, \underline{h(\bar{g}k)}\, B(\bar{g})$$

Particularly interesting case is when we fix k_* and look at $G_{k_*} = \{\{\bar{g}|\vec{d}\} \mid \bar{g}k_* = k_* + \vec{b}_{\bar{g}} \text{ for } \vec{b}_{\bar{g}} \in \Upsilon\}$

$$g \in G_{k_*} \quad u_g|\chi_{a k_*}\rangle = \sum_b |\chi_{b \bar{g} k_*}\rangle B_{ba}(\bar{g}) e^{-i\bar{g}k_* \cdot \vec{d}}$$

$$= \sum_b |\chi_{c k_*}\rangle V_{cb}(\vec{b}_g) B_{ba}(\bar{g}) e^{-i\bar{g}k_* \cdot \vec{d}}$$

$$\boxed{\begin{gathered} \rho_*: \underset{\substack{\cup \\ g}}{G_{k_*}} \to V(\vec{b}_g) B(\bar{g}) e^{-i\bar{g}k_* \cdot \vec{d}} \quad \text{defines a representation of the little group } G_{k_*} \\ [V(\vec{b}_g) B(\bar{g}) e^{-i\bar{g}k_* \cdot \vec{d}}, \underbrace{h(k_*)}_{\text{tight-binding Hamiltonian matrix}}] = 0 \end{gathered}}$$

A Band representation determines all the little group irreps for Bands in the BZ

Berry connection in the tight-binding basis

starting point (approximate) eigenstates $|\psi_{nk}\rangle \simeq \sum_a u^a_{nk} |\chi_{ak}\rangle$

$$u_{nk}(\vec{r}) = e^{-ik\cdot\vec{r}} \langle \vec{r} | \psi_{nk} \rangle = \sum_a u^a_{nk} e^{-ik\cdot r} \boxed{\langle r | \chi_{ak} \rangle}$$

$$= \sum_{a\vec{R}} u^a_{nk} e^{ik\cdot(R + \bar{r}_a - \vec{r})} W_{aR}(\vec{r})$$

Berry connection:

$$A^{nm}_i(k) = i \left\langle u_{nk} \middle| \frac{\partial u_{mk}}{\partial k_i} \right\rangle_{cell} = i \int d^3y\, u^*_{nk}(y) \frac{\partial u_{mk}(y)}{\partial k_i}$$

$$= i\int_{\text{cell}} d^3y \sum_{\substack{ab \\ RR'}} \left[u^a_{nk} e^{ik\cdot(R+\bar{r}_a-\bar{y})} W_{aR}(y)\right]^* \frac{\partial}{\partial k_i}\left[u^b_{mk} e^{ik\cdot(R'+\bar{r}_b-y)} W_{bR'}(y)\right]$$

$$= i\int_{\text{cell}} d^3y \sum_{\substack{ab \\ RR'}} e^{ik\cdot(R'+\bar{r}_b-R-\bar{r}_a)} W^*_{aR}(y) W_{bR'}(y)\left[\underbrace{(u^a_{nk})^* \frac{\partial u^b_{mk}}{\partial k_i}}_{1} + \underbrace{u^{a*}_{nk} u^b_{mk}(R'+\bar{r}_b-y)}_{2}\right]$$

$$1 \quad i\int_{\text{cell}} d^3y \sum_{ab} \chi^*_{ak}(y)\chi_{bk}(y)(u^a_{nk})^* \frac{\partial u^b_{mk}}{\partial k_i} = i\,\vec{u}^{\,\dagger}_{nk}\cdot \frac{\partial \vec{u}_{mk}}{\partial k_i} \leftarrow \text{tight-binding Berry connection}$$

$$2 \quad \sum_{RR'} e^{ik\cdot(R'-R+\bar{r}_b-\bar{r}_a)}\int_{\text{cell}} dy\, W^*_{aR}(y)\left[R'+\bar{r}_b-y\right] W_{bR'}(y) \qquad R''=R'-R$$

$$\sum_{R''} e^{ik\cdot(R''+\bar{r}_b-\bar{r}_a)} \sum_{R'} \int_{cell} d^3y \, W^{+}_{aR'-R''}(y) \left[R'+\bar{r}_b-y\right] W_{bR'}(y)$$

$$= \sum_{R''} e^{ik\cdot(R''+\bar{r}_b-\bar{r}_a)} \sum_{R'} \int_{cell} d^3y \, W^{+}_{a-R''}(y-R')\left[\bar{r}_b-[y-R']\right] W_{b0}(y-R')$$

$$= \sum_{R''} e^{ik\cdot(R''+\bar{r}_b-\bar{r}_a)} \int_{space} d^3\vec{r} \, W^{+}_{a-R''}(\vec{r})\left[\bar{r}_b-\vec{r}\right] W_{b0}(\vec{r})$$

$$= \delta_{ab}\bar{r}_b - \sum_{R''} e^{ik\cdot(R''+\bar{r}_b-\bar{r}_a)} \langle W_{a-R''} | \vec{x} | W_{b0} \rangle$$

useful approximation: very localized wannier functions

$$\rightarrow \quad \langle W_{aR} | \vec{x} | W_{bR'} \rangle \approx \delta_{ab}\, \delta_{RR'} (R + \bar{r}_a)$$

$$\boxed{\langle W_{aR} | e^{i k \cdot \vec{x}} | W_{bR'} \rangle \overset{?}{\not\approx} \delta_{ab}\, \delta_{RR'}}$$

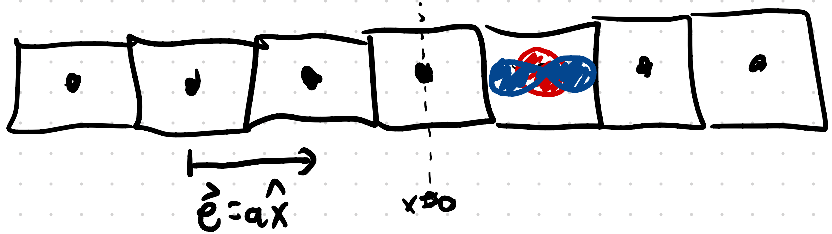
"strict tight-binding limit"

in this approximation ② = 0

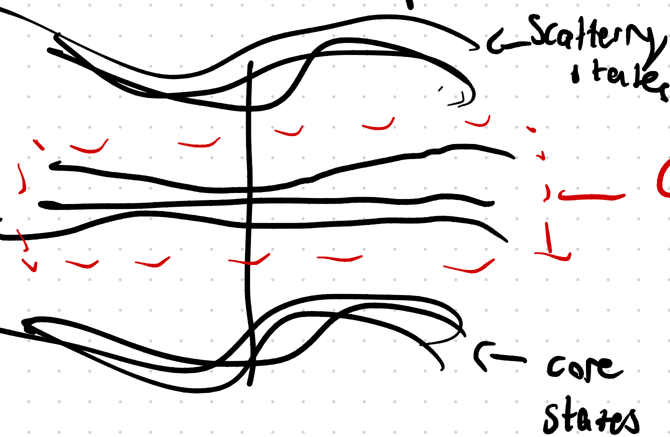
$$A_i^{nm}(k) \longrightarrow i\, \vec{u}_{nk}^{\dagger} \cdot \frac{\partial \vec{u}_{mk}}{\partial k_i}$$

In the strict tb limit $h(k)$, E_{nk}, $A_i(k)$ depend on the centers of the Wannier functions, but not on their shape

Example: 1d chain w/ inversion & time reversal symmetry



$$p\bar{1}1' = \langle \{E|a\hat{x}\}, \{I|0\}, T \rangle$$

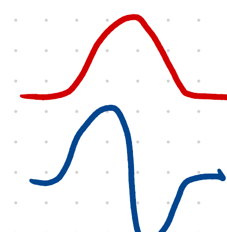


come from valence electrons on the atoms

Tight binding basis function

$|W_{sR}\rangle$ - s like orbital

$|W_{p\vec{R}}\rangle$ - p-like orbital



$i,j = s,p$

$$\langle W_{i\vec{R}} | W_{j\vec{R}'} \rangle = \delta_{ij}\,\delta_{RR'}$$

tb limit

$$\langle W_{i\vec{R}} | x | W_{j\vec{R}'} \rangle = \delta_{ij}\,\delta_{RR'}\,R$$

Ignore spin

Inversion symmetry:

$$W_{s\vec{0}}(-x) = W_{s\vec{0}}(x)$$
$$W_{p\vec{0}}(-x) = -W_{p\vec{0}}(x)$$

$$u_{\{I|0\}} |W_{i\vec{R}}\rangle = \sum_j |W_{j\,-R}\rangle\, B_{ji}(I)$$

$$B_{ji}(I) = \begin{array}{c c} & \begin{array}{cc} s & p \end{array} \\ \begin{array}{c} s \\ p \end{array} & \begin{pmatrix} +1 & 0 \\ 0 & -1 \end{pmatrix} \end{array} = \sigma^z_{ij}$$

$$w_{iR}^{*}(x) = w_{iR}(r) \rightarrow B_{ij}(T) = \sigma_{ij}^{\circ} \mathcal{K}$$

Localized WFs → look for "nearest neighbor" TB model

$$\langle w_{iR} | H | w_{jR'} \rangle = \begin{cases} \varepsilon_{ij}, & R = R' \\ t_{ij}, & R = R' + a \\ t_{ji}^{*} & R = R' - a \quad \leftarrow \text{hermiticity} \\ 0 & \text{otherwise} \end{cases}$$

$$\parallel$$

$$h^{ij}(R - R')$$

$$h^{ij}(R-R') = \varepsilon_{ij} \delta_{RR'} + t_{ij} \delta_{R,R'+a} + t_{ji}^{*} \delta_{R,R'-\vec{a}}$$

$$h^{ij}(k) = \sum_R e^{-ik\cdot R} h^{ij}(R) = \varepsilon_{ij} + t_{ij} e^{-ik\cdot a} + t^*_{ji} e^{ik\cdot a}$$

$$B(\bar{g})^{-1} h(\bar{g}k) B(\bar{g}) = h(k)$$

TRS: $B(T) = \sigma^0_{ij} \mathcal{K} \Rightarrow h^*(-k) = h(k)$

$$\varepsilon^*_{ij} = \varepsilon_{ij}$$

$$t_{ij} = t^*_{ij}$$

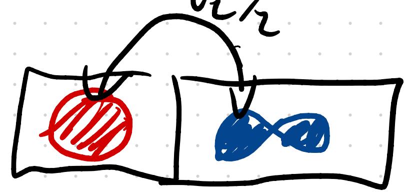
Inversion: $B(I) = \sigma^z_{ij}$

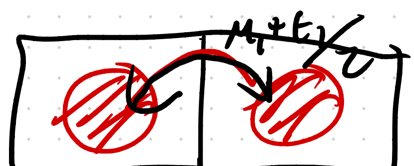
$$\sigma^z h(-k)\sigma^z = h(k)$$

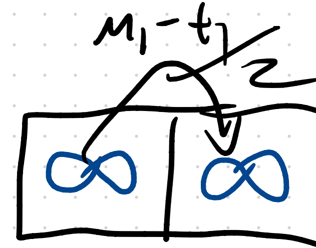
$$[\sigma^z, \varepsilon_{ij}] = 0 \qquad \varepsilon_{ij} = \mu\sigma^0_{ij} + \Delta\sigma^z_{ij}$$

$$\sigma_z t_{ij}\sigma_z = t^*_{ji} = t_{ji} \qquad t_{ij} = \frac{\mu_1}{2}\sigma^0_{ij} + \frac{t_1}{2}\sigma^z_{ij} - \frac{it_2}{2}\sigma^y_{ij}$$

$$h(k) = \sigma^0_{ij}(\mu + \mu_1\cos ka) + (\Delta + t_1\cos ka)\sigma^z_{ij} + t_2\sin ka\,\sigma^y_{ij}$$







Finding the energies:

$$d_0(k) = \mu + \mu_1 \cos ka$$

$$d_z(k) = \Delta + t_1 \cos ka$$

$$d_y(k) = t_2 \sin ka$$

$$h_{ij}(k) - d_0(k)\sigma^0_{ij} = d_z(k)\sigma^z_{ij} + d_y(k)\sigma^y_{ij}$$

$\mu, \nu = x, y, z$

$$\{\sigma^\mu, \sigma^\nu\} = \sigma^\mu\sigma^\nu + \sigma^\nu\sigma^\mu$$
$$= 2\delta_{\mu\nu}\sigma^0$$

$$\left[h(k) - d_0(k)\sigma^0_{ij}\right]^2 = \sum_{\alpha\beta = z,y} d_\alpha(k) d_\beta(k) \sigma^\alpha \sigma^\beta$$

$$= \left(d_z^2(k) + d_y^2(k) \right) \sigma_0$$

$$\varepsilon_\pm(k) = d_0(k) \pm \sqrt{d_z^2(k) + d_y^2(k)}$$ are the eigenvalues of $h(k)$

$$\boxed{\varepsilon_\pm(k) = \mu + \mu_1 \cos ka \pm \sqrt{(\Delta + t_1 \cos ka)^2 + t_1^2 \sin^2 ka}}$$