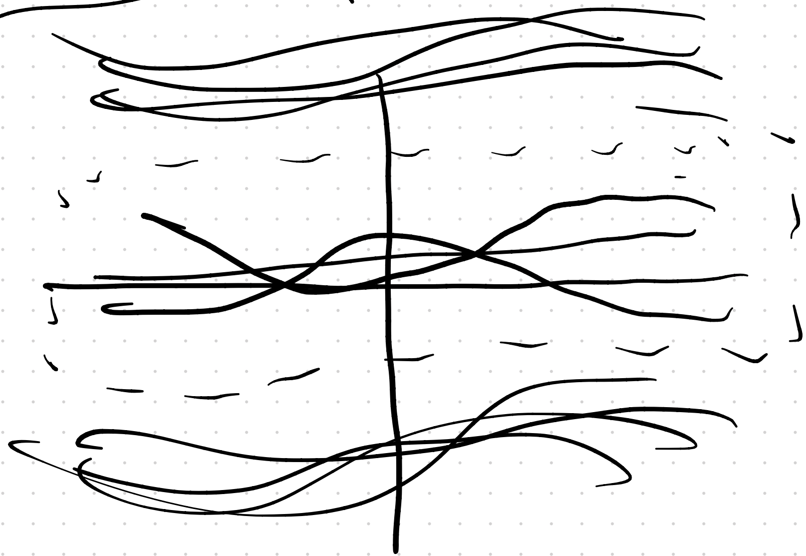
Lecture 19

Reminder: Send final presentation topic ideas by 4/8



Wannier functions

$|W_{a\vec{R}}\rangle$ centered at $\vec{R}+\vec{r}_a$

tight-binding basis fns $|\chi_{a\vec{k}}\rangle = \sum_{\vec{R}} e^{i\vec{k}\cdot(\vec{R}+\vec{r}_a)} |W_{a\vec{R}}\rangle$

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

we can truncate to obtain

approximations

(approximate) eigenstate $|\psi_{nk}\rangle = \sum_a u^a_{nk} |\chi_{ak}\rangle$

Schrödinger Eqn: $h(k)\vec{u}_{nk} = E_{nk}\vec{u}_{nk}$ - finite dim matrix equation

$\vec{G} \in \check{T}$ a reciprocal lattice vector

$$|\chi_{ak+\vec{G}}\rangle = V_{ab}(\vec{G})|\chi_{bk}\rangle$$

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

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

"embedding matrix"

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

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

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

representation of pt grp $\bar{G} = G/T$

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

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

Particular case: fix k_*, look @ little group

$$G_{k_*} = \{\{\bar{g}|\vec{d}\} \mid \bar{g}k_* \equiv k_* \bmod \check{T}\}$$

for $g \in G_{k_*}$, $\quad \bar{g}k_* = k_* + \vec{b}_g \quad \vec{b}_g \in \check{T}$

$$U_g|\chi_{ak_*}\rangle = \sum_b |\chi_{b\,\bar{g}k_*}\rangle B_{ba}(\bar{g}) e^{-i\bar{g}k_*\cdot\vec{d}}$$

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

Band representation determines a little grp rep

$$\rho_{\vec{k}}: \underset{\substack{\cap \\ G_{k_*}}}{g} \to V(\vec{b}_g) B(\bar{g}) e^{-i\bar{g}k_*\cdot\vec{d}}$$

representation of $G_{\vec{k}}$

$$[V(\vec{b}_g) B(\bar{g}) e^{-i\bar{g}k_*\cdot\vec{d}}, h(k_*)] = 0$$

Band representation determines all little grp representations for bands in the BZ

Berry connection in the tight-binding basis

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

$$\langle \vec{r} | \psi_{nk} \rangle = e^{i k \cdot \vec{r}} u_{nk}(\vec{r})$$

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

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

Berry connection

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

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

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

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

$$2 \; -\int_{cell} d^3y \sum_{RR'} e^{i\vec k\cdot(R'+\bar r_b-R-\bar r_a)}\, W^{*}_{aR}(y)\,[R'+\bar r_b-y]_i\, W_{bR'}(y)$$

$$R'' = R' - R$$

$$= -\sum_{R''} e^{ik\cdot(R''+\bar r_b-\bar r_a)} \sum_{R'} \int_{cell} d^3y\; W^{*}_{aR'-R''}(y)\,[R'+\bar r_b-y]_i\, W_{bR'}(y)$$

$$W_{bR'}(y) = W_{b0}(y-R')$$

$$W_{aR'-R''}(y) = W_{a,-R''}(y-R')$$

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

$$\vec{r} = y - R'$$

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

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

useful approximation: very-localized Wannier fns

$$\langle W_{a\,-R''} | x_i | W_{b0} \rangle \approx \delta_{ab}\, \delta_{R'',0}\, \bar{r}_b$$

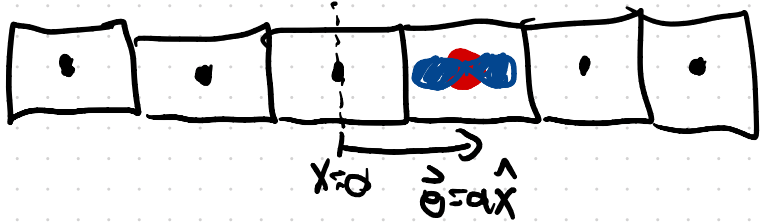
"strict" tight-binding limit

in this approximation (2) = 0

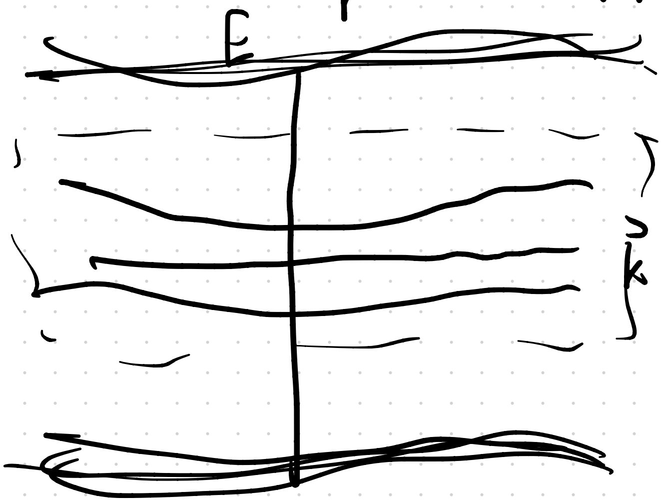
$$A_i^{nm}(\vec{k}) \longrightarrow i\, \vec{u}_{nk}^{\dagger} \cdot \frac{\partial \vec{u}_{mk}}{\partial k_i}$$

$h(k)$, E_{nk}, u_{nk}^{a}

Example: 1d crystal w/ inversion symmetry & time-reversal symmetry



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

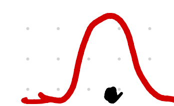


come from the valence s and p orbitals

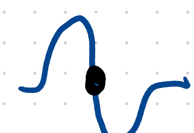
i, j = s or p

Tight-binding basis functions

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



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



$$\langle W_{iR} | W_{jR'} \rangle = \delta_{ij}\, \delta_{RR'}$$

strict tb limit

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

Inversion: $\{I|0\}\, \vec{x} = -\vec{x}$

$$W_{so}(x) \to W_{so}(-x) = W_{so}(x)$$

$$W_{p\alpha}(x) \to W_{p\alpha}(-x) = -W_{p\alpha}(x)$$

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

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

Time-reversal symmetry (ignore spin): take $W_{iR}(x)$ to be real $B_{ij}(T) = \sigma^0_{ij} K$

σ^0: identity matrix

Localized WFs → look for "nearest-neighbor" tb model

$$\underline{h^{ij}(R-R')} = \langle W_{iR} | H | W_{jR'} \rangle = \begin{cases} \varepsilon_{ij} & \text{if } R = R' \\ t_{ij} & R = R' + a \end{cases}$$

$$\begin{cases} t_{ji}^{*} & R = R' - a \\ 0 & \text{otherwise} \end{cases}$$

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

$$h^{ij}(k) = \sum_{R} e^{-ik\cdot R}\, h^{ij}(R) = \varepsilon_{ij} + e^{-ika}\, t_{ij} + e^{ika}\, t_{ji}^{*}$$

Symmetries give us constraints on ε_{ij}, t_{ij}

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

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

$$\Rightarrow \varepsilon^*_{ij} + e^{-ika} t^*_{ij} + e^{ika} t_{ji} = \varepsilon_{ij} + e^{-ika} t_{ij} + e^{ika} t^*_{ij}$$

$$\Rightarrow \boxed{\begin{aligned} \varepsilon_{ij} &= \varepsilon^*_{ij} \\ t_{ij} &= t^*_{ij} \end{aligned}}$$

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

$$\sigma_z h(-k) \sigma_z = h(k)$$

$$\sigma_z \varepsilon \sigma_z + e^{ika} \sigma_z t \sigma_z + e^{-ika} \sigma_z t^\dagger \sigma_z = \varepsilon_{ij} + e^{-ika} t + e^{ika} t^\dagger$$

$$\sigma_z \varepsilon \sigma_z = \varepsilon \Rightarrow [\sigma_z, \varepsilon] = 0 \qquad \varepsilon^\dagger = \varepsilon$$

$$\sigma_z t \sigma_z = t^\dagger = t^T$$

$\sigma^0 \quad \sigma^x \quad \sigma^y \quad \sigma^z$

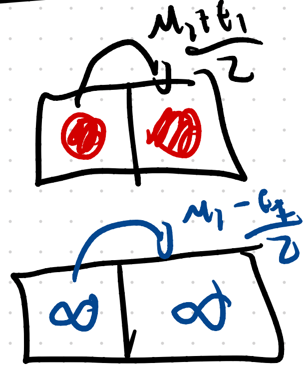
real, symmetric

imaginary, antisymmetric

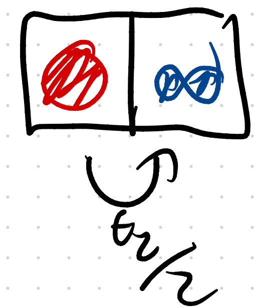
$$\Rightarrow \varepsilon_{ij} = \mu \sigma^0_{ij} + \Delta \sigma^z_{ij}$$

$$\Rightarrow t_{ij} = \frac{\mu_1}{2} \sigma^0_{ij} + \frac{t_1}{2} \sigma^z_{ij} - \frac{it_2}{2} \sigma^y_{ij}$$

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



on-site energy splitting between s & p



Finding energies:

$$d_0(k) = \mu + \mu_1 \cos ka$$
$$d_z(k) = \Delta + t_1 \cos ka$$
$$d_y(k) = t_2 \sin ka$$

$$h(k) - d_0 \sigma^0 = d_z \sigma^z + d_y \sigma^y$$

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

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

$$(\sigma^\mu)^2 = \sigma^0$$

$$\left(h(k) - d_0 \sigma^0\right)^2 = \left(d_z^2 + d_y^2\right) \sigma^0$$

Eigenvalues of H satisfy $\left(\varepsilon_\pm(k) - d_0\right)^2 = \left(d_z^2 + d_y^2\right)$

$$\varepsilon_\pm(k) = d_0(k) \pm \sqrt{d_z^2(k) + d_y(k)^2}$$

$$\Rightarrow \boxed{\varepsilon_\pm(k) = \mu + \mu_1 \cos ka \pm \sqrt{(\Delta + t_1 \cos ka)^2 + t_2^2 \sin^2 ka}}$$