

## Lecture 21

- Reminder: Send me your final presentation preferences by Thurs.
- HW Posted, due 4/17
- Solutions to HW 2 are posted

Last time, we introduced the tight-binding Hamiltonian

$$h^{ab}(\vec{k}) = \sum_R \langle w_{aR} | [H] | w_{bR} \rangle e^{-i\vec{k}_a \cdot (R + \vec{r}_a - \vec{r}_b)}$$

where  $[H]$  denotes some systematic (symmetric)

translation of  $H$  in position space

$$\text{i.e. } [H] = \int dx dx' |x\rangle \langle x| H |x'\rangle \langle x'| \\ \theta(\Delta - |\vec{x} - \vec{x}'|)$$

We will assume that  $\{|w_{\alpha R}\rangle\}$ ,  $[H]$  (and therefore  $h^{ab}(k)$ ) transform under the same space group as  $H$

$$|\psi_{nk}\rangle \approx \sum_a u_{nk}^a |\chi_{ak}\rangle$$

where

$$|\chi_{ak}\rangle = \sum_R e^{ik \cdot (R + \bar{r}_a)} |w_{aR}\rangle$$

If

$$h(k) \vec{u}_{nk} = E_{nk} \vec{u}_{nk}$$

then

right-brady  
eigenvectors

$$H |\psi_{nk}\rangle = E_{nk} |\psi_{nk}\rangle$$

$H$  is symmetric under some space group  $G$ , and  $\{|w_{aR}\rangle\}$  transforms as a representation of  $G$

$$g = \{\hat{g} | \hat{d}\} \in G$$

$$[H] = \sum_{abRR'} |w_{aR} \times w_{aR'} \langle H | w_{bR} \times w_{bR'}| \times \Theta(K_w aR |H| w_{bR'}) - S)$$

$$W'_{aR}(r) = \langle r | U_g | W_{aR} \rangle = W_{aa}(g^{-1}r) = W_a(g^{-1}r - R - \bar{r}_a)$$

Now lets use the following facts:

$$\begin{aligned} \langle g^{-1}r | W_{aR} \rangle &= W_{aR}(r) = W_{a0}(r - R) \\ &= W_a(r - R - \bar{r}_a) \end{aligned}$$

$$\begin{aligned} W_{aR}(g^{-1}r) &= W_a(g^{-1}r - R - \bar{r}_a) \\ &= W_a(g^{-1}(r - gR - g\bar{r}_a)) \\ &= W_b(r - R' - \bar{r}_b) B_{ba}(y) \end{aligned}$$

$$\Rightarrow R' = g(R - \bar{r}_a) - \bar{r}_b$$

$$V_g |W_{aR}\rangle = \sum_b W_{bR'}(r) \beta_{ba}(g) S_{R', g(R-\bar{r}_a) - \bar{r}_b}$$

$\beta(g)$  form a representation of the space group

$$F \quad g = \{E|\vec{t}\}$$

$$W_{aR}(g^{-1}\vec{r}) = V_{aR}(\vec{r} - \vec{t}) = W_{aR+\vec{t}}(r)$$

$$R' = g(R - r_a) - r_q = R + \vec{t}$$

$$\Rightarrow B(\{e|\vec{t}\}) = S_{ab}$$

$\Rightarrow$   $B$  is a representation of the space group induced from  $\Gamma$  (all lattice translations are represented trivially)

$B(\{\bar{g}|\vec{d}\}) = B(\bar{g})$  is a point group representation

Summary  $\sum_{\{g|\vec{d}\}} |W_{gR}\rangle = \sum_{bR} |W_{bR}\rangle \otimes B_{ba}(g)$

$$+ S_{R(g(R-\vec{t}))} \vec{f}$$

We can Fourier transform this to see  
how symmetries act on  $|X_{ab}\rangle$

KCHG6

$\gamma: H \rightarrow U(V)$  is a representation

s.t.  $\gamma(k) = \text{Id} \quad \forall k \in K$

$$\gamma \circ G(k) \stackrel{?}{=} \text{Id}$$

$$\begin{aligned} O_{\{\vec{g}\}} |X_{ak}\rangle &= \sum_R O_{\{\vec{g}\}} |W_{aR}\rangle e^{ik \cdot (R + \vec{r}_a)} \\ &= \sum_{RR'} e^{ik \cdot (R + \vec{r}_a)} |W_{bR'}\rangle B_{ba}(g) S_{R', \vec{g}(R + \vec{r}_a) - \vec{r}_b} \end{aligned}$$

$$= \sum_{R'} e^{ik \cdot (\bar{g}^{-1}(R' + \bar{r}_b - \bar{r}) - \bar{k}_q + \bar{k}_a)} \\ |W_{bR'} > B_{ba}(g)$$

$$= e^{-ik \cdot \bar{g}^{-1}\bar{r}} \sum_{R'} e^{i\bar{k} \cdot \bar{g}^{-1}(R' + \bar{r}_b)} |W_{bR'} > \cancel{B_{ba}(g)}$$

Since  $\bar{g}$  is a point grp operation

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

$$k \cdot \bar{g}^{-1} d = (\bar{g} k) \cdot \bar{d}$$

$$k \cdot \bar{g}^{-1} (R' + \bar{r}_b) = \bar{g} k \cdot (R' + \bar{r}_b)$$

$$\left\langle \sum_{\{\bar{g}\}} |\chi_{ak}\rangle \right| = e^{-i(\bar{g}k) \cdot \bar{d}} \sum_{R'} e^{i\bar{g}k \cdot (R' + \bar{r}_b)} \langle W_{bR'} | \chi_{ba}(S) | \chi_{b\bar{g}k} \rangle$$

$$U_{\{\bar{g}\} \rightarrow \{x_{ak}\}} |x_{ak}\rangle = |x_{b\bar{g}k}\rangle B_{ba}(g) e^{-i(\bar{g}k)\cdot \vec{p}}$$

$$B: G \rightarrow U(N)$$

$$B(\{E|\vec{e}\}) = \text{id}$$

$$G/\tau = \overline{G}$$

$$\hat{h}(k) = \langle x_{ak} | L^H | x_{bk} \rangle$$

$$[H, U_g] = 0 \quad \forall g \in G$$

$$h^{ab}(k) = \langle X_{ak} | U_g^\dagger [H] U_g | X_{bk} \rangle$$

$$= e^{i\vec{g} \cdot \vec{k}} B_{ac}^+ \langle X_{c\bar{g}k} | [H] | X_{d\bar{g}k} \rangle B_{db}^- e^{-i\vec{g} \cdot \vec{k}}$$

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

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

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

$$\text{if } \hat{g}k \in k + G_g$$

$$\begin{aligned} \text{then } h(k) &= B^+(g) h(k+G_g) B(g) \\ &= B^+(g) V^+(G_g) h(k) V(G_g) B(g) \end{aligned}$$

$$\Rightarrow [V(G_g)B(g)e^{\frac{-igk\cdot d}{\hbar}}h(k)] = 0$$

$$\{ V(G_g)B(g)e^{\frac{-igk\cdot d}{\hbar}}g_k = k + G_g \} \text{ form}$$

a representation of the little grp  $G_k$   
in the tight-binding basis

Lets turn to the Berry connection in the  
tight-binding basis

$$|\Psi_{nk}\rangle = \sum_a |u_{nk}^a | \chi_{ak} \rangle$$

$$\begin{aligned} u_{nk}(r) &\equiv \sum_a u_{nk}^a \chi_{ak}(r) e^{-ik \cdot r} \\ &= \sum_{aR} u_{nk}^a e^{ik \cdot (R + \bar{r}_a - r)} w_{ak}(r) \end{aligned}$$

tight-binding approx to cell periodic  
 $u_{nk}(r)$

Let's evaluate  $A_m^{nn}(k) = i \langle u_{nk} | \partial_m u_{nk} \rangle$  in  
the fb approximation

$$A_m^{nn}(k) = \int d^3r i u_{nk}(r) \partial_m u_{nk}(r)$$

cell

$$\approx i \int d^3r \sum_{aR} \sum_{bR'} (U_{nk}^a)^* e^{-ik \cdot (R + r_a - r)} W_{aR}^*(r)$$

cell

$$\times \frac{\partial}{\partial k_m} \left[ U_{mk}^b e^{ik \cdot (R' + r_b - r)} W_{bR'}(r) \right]$$

$$= i \int_{\text{cell}} d^3r \sum_{\substack{aR \\ bR'}} e^{ik \cdot (R' + \bar{r}_b - R - \bar{r}_a)} W_{aR}^*(\bar{r}) W_{bR'}(r) (U_{nk}^a)^* \left[ \begin{array}{l} \textcircled{1} \\ \partial_m U_{mk}^b \end{array} \right] \\ + i U_{mk}^b (R' + r_b - r) \quad \textcircled{2}$$

$$\textcircled{1} \quad i \int_{\text{cell}} d^3r X_{ak}^*(r) X_{bk}(r) (U_{nk}^a)^* \partial_m U_{mk}^b \\ = i (U_{nk}^a)^* \partial_m U_{mk}^a = i \tilde{U}_{nk}^+ \cdot \partial_m \tilde{U}_{mk}$$

Berry connection of tight-binding  
eigenvectors

② Not so nice

$$\sum_{\substack{R R' \\ ab}} U_{nk}^{ra} U_{mk}^b e^{ik \cdot (R' - R + \bar{r}_b - \bar{r}_a)} \int_{\text{cell}} dr W_{aR}^+(r) [R' + \bar{r}_b - r] W_{bR}(r)$$

$$y = r - R'$$

$$R' = R - R'$$

$$= \sum_{\substack{R'' \\ ab}} U_{nk}^{a*} U_{mk}^b e^{ik \cdot (\bar{r}_b - \bar{r}_a - R'')} \int dy W_{aR''}^*(y) [\bar{r}_b - y] W_{b0}(y)$$

Space

if we use

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

Useful approximation:  $\langle W_{aR} | \vec{x} | W_{bR'} \rangle = S_{ab} S_{RR'} \langle \vec{r}_a \rangle$

$\uparrow$   
(strict) tight - binding limit

→ ② vanishes in the t.b. limit

$$A_m^M(k) \xrightarrow{\text{tight-binding limit}} i \vec{U}_{mk}^\dagger \partial_m \vec{U}_{mk}$$

This means that as long as

$$\langle W_{aR} | \vec{x} | W_{bR'} \rangle \leq S_{ab} S_{R R'} F_a$$

then we can "forget everything about  $|W_{aR}\rangle$   
except for their centers and still approximate

$h(k)$ ,  $E_{nk}$ , and  $A_m(k)$

If  $W_{ar}(r) \sim e^{-|r-R|/\xi}$  at large distances

then if  $\xi \ll$  lattice constant

$$\langle W_{ar} | \hat{x} | W_{bR} \rangle = S_{ab} S_{RR'} \bar{r}_b + O(e^{-|R-R'|/\xi})$$