Lecture 18

- Email final presentation topic idea to me by 4/8
- HW 3 due tonight
- HW4 posted, due 4/10

Recap $\langle \psi_{nk} | [Px_iP, Px_jP] | \psi_{mk'} \rangle = \frac{(2\pi)^3}{v} \delta(k-k') \, i \, \Omega_{ij}^{nm}(k)$

Berry Curvature $\Omega_{ij}^{nm}(k) = \left(\left[\frac{\partial A_j}{\partial k_i} - \frac{\partial A_i}{\partial k_j} - i [A_i, A_j] \right] \right)^{nm}$

$\rightarrow$ Exponentially localized WF $|W_{n\vec{R}}\rangle$ are <u>not</u> simultaneous eigenfunctions $P\vec{x}P$

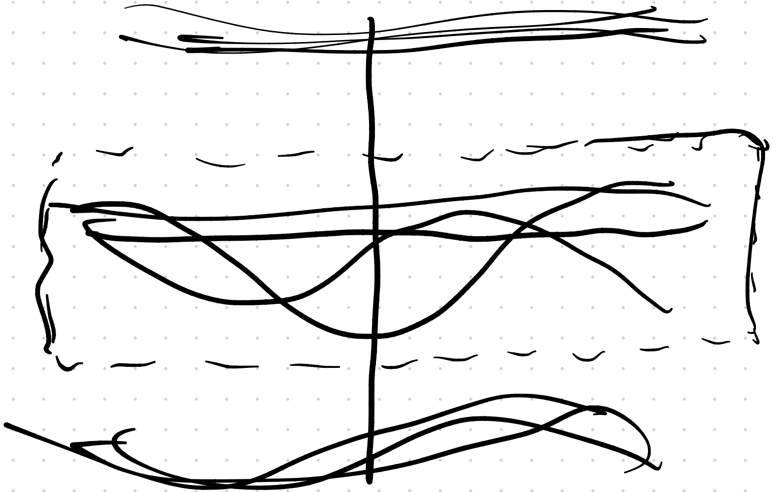
→ Obtained via numerical minimization

$$\langle W_{a\vec{R}} | W_{bR'} \rangle = \delta_{ab} \, \delta_{RR'}$$

$$U_{\vec{t}} | W_{a\vec{R}} \rangle = | W_{aR+\vec{t}} \rangle \text{ for } \vec{t} \in T$$

$$W_{a\vec{R}}(\vec{r}) = \langle \vec{r} | W_{a\vec{R}} \rangle = \langle r | U_{\vec{R}} | W_{a\vec{0}} \rangle = W_{a\vec{0}}(\vec{r} - \vec{R})$$

1. When can we find $\{ | W_{a\vec{R}} \rangle \}$
2. What can we do with them



Spectrum of Hamiltonian H

P projects onto these N "low energy bands"

$\rightarrow$ assume we find some $\{|W_{aR}\rangle\}$

$$\langle W_{aR}|H|W_{bR'}\rangle$$

H has discrete translation symmetry

$$\begin{aligned}&\langle W_{aR}|H|W_{bR'}\rangle \\ &= \langle W_{aR}|H U_{R'}|W_{b\vec{0}}\rangle = \langle W_{aR}|U_{R'} H|W_{b\vec{0}}\rangle = \langle W_{aR-R'}|H|W_{b0}\rangle \\ &\equiv h^{ab}(\vec{R}-\vec{R}')\end{aligned}$$

$h^{ab}(\vec{R}-\vec{R}')$ – tight binding Hamiltonian

$\Big\{$ $N \times N$ matrix

We can now Fourier transform h

Wannier centers $\langle W_{a\vec{R}} | \vec{x} | W_{a\vec{R}} \rangle = \vec{R} + \bar{r}_a$

Tight binding basis functions $|\chi_{a\vec{k}}\rangle = \sum_{\vec{R}} e^{ik\cdot(R+\bar{r}_a)} |W_{a\vec{R}}\rangle$

$$|W_{a\vec{R}}\rangle = \frac{v}{(2\pi)^3} \int d^3k \, |\chi_{a\vec{k}}\rangle e^{-ik\cdot(R+\bar{r}_a)} \qquad = e^{ik\cdot\bar{r}_a} |\tilde{\varphi}_{a\vec{k}}\rangle$$

$\underline{h^{ab}(R-R')} = \langle W_{aR} | H | W_{bR'} \rangle$

$$= \left(\frac{v}{(2\pi)^3}\right)^2 \int d^3k\, d^3k' \underbrace{\langle \chi_{ak} | H | \chi_{bk'} \rangle}_{[H, u_e] = 0} e^{i(k\cdot(R+r_a) - k'\cdot(R'+r_b))}$$

Schur's lemma $\rightarrow \langle \chi_{ak} | H | \chi_{bk'} \rangle = 0$ if $k \neq k'$

$$\langle \chi_{ak} | H | \chi_{bk'} \rangle = \frac{(2\pi)^3}{v} \delta(k-k') \langle \chi_{ak} | H | \chi_{bk} \rangle$$

$$h^{ab}(R-R') = \frac{v}{(2\pi)^3} \int d^3k \left[e^{ik\cdot r_a} \langle \chi_{ak} | H | \chi_{bk} \rangle e^{-ik\cdot r_b} \right] \underline{e^{ik\cdot(R-R')}}$$

$$\boxed{h^{ab}(\vec{k}) = \langle \chi_{ak} | H | \chi_{bk} \rangle}$$

$$h^{ab}(R) = \frac{v}{(2\pi)^3} \int dk \left(e^{ik\cdot r_a} h^{ab}(k) e^{-ik\cdot r_b} \right) e^{ik\cdot R}$$

$$\boxed{V_{ab}(\vec{k}) = e^{i k \cdot \bar{r}_a} \delta_{ab}} \text{ - Embedding matrix}$$

$$\boxed{h^{ab}(R) = \frac{v}{(2\pi)^3} \int dk \left[V(k) h(k) V^{\dagger}(k) \right]^{ab} e^{i k \cdot R}}$$

$$|\chi_{a k+\vec{G}}\rangle = \sum_R e^{i(k+G)\cdot(R+\bar{r}_a)} |W_{aR}\rangle \qquad |\chi_{a\vec{k}}\rangle = \sum_{\vec{R}} e^{ik\cdot(R+\bar{r}_a)} |W_{a\vec{R}}\rangle$$

$$= e^{iG\cdot \bar{r}_a} |\chi_{a\vec{k}}\rangle$$

$$= \sum_b V_{ab}(G) |\chi_{bk}\rangle \quad \text{for } G \in \check{T} \text{ in the reciprocal lattice}$$

$$h^{ab}(k+G) = \langle \chi_{ak+G} | H | \chi_{bk+G} \rangle = \left[V^{\dagger}(G)\, h(k)\, V(G) \right]^{ab}$$

How this is useful: Expand eigenstates of H in terms of $|\chi_{ak}\rangle$

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

$$P|\psi_{nk}\rangle = |\psi_{nk}\rangle$$

$$|\psi_{nk}\rangle = \sum_{a=1}^{N} |\chi_{a\vec{k}}\rangle u^{a}_{nk}$$

u^{a}_{nk} is a vector of coefficients indexed by $a = 1, \ldots N$

$$\langle \chi_{ak} | H | \psi_{nk} \rangle = E_{nk} \langle \chi_{ak} | \psi_{nk} \rangle$$

$$\sum_{b=1}^{N} \langle \chi_{ak} | \overset{H}{H} | \chi_{bk} \rangle u_{nk}^{b} = E_{nk} u_{nk}^{a}$$

$$\boxed{\begin{aligned} h(k) \vec{u}_{nk} &= E_{nk} \vec{u}_{nk} \\ \vec{u}_{nk+G} &= V^{\dagger}(G) \vec{u}_{nk} \end{aligned}}$$

← $N \times N$ matrix equation <u>equivalent</u> to Schrödinger equation on our N bands of interest.

Basis for approximation: $h^{ab}(R-R') = \langle W_{aR} | H | W_{bR'} \rangle$

if $|W_{aR}\rangle$ are exponentially localized

then we expect

$$h^{ab}(R-R') \sim e^{-|R-R'|/\xi} \quad \text{for } |R-R'| \text{ large}$$

Pick $\Delta \sim O(\xi)$ $\quad e^{-\Delta/\xi}$ is small enough that we can ignore it

$$h^{ab}(R-R') \rightarrow \lfloor h^{ab}(R-R') \rfloor = \begin{cases} h^{ab}(R-R'), & |R-R'| < \Delta \\ 0 & |R-R'| > \Delta \end{cases}$$

<u>Tight binding approximation</u>

Lets return to space group symmetries

H is invariant under a space grp G $\quad \{|\psi_{nk}\rangle\}$

transform in representations of G

We want WFs $\{|W_{a\vec{R}}\rangle\}$ to also transform in representations of G

always true $\rightarrow$ ① $\{|W_{aR}\rangle\}$ form a representation of $T \triangleleft G$

$$U_t |W_{a\vec{R}}\rangle = |W_{aR+\vec{t}}\rangle$$

$$|W_{a\vec{R}}\rangle = \frac{V}{(2\pi)^3}\int d^3k\, e^{-ik\cdot R}|\psi_{ak}\rangle$$

② $\langle r|W_{a\vec{R}}\rangle \equiv W_{a\vec{R}}(r)$ centered at $R+\overline{r_a}$

$$W_{a\vec{R}}(\vec{r}) = W_{a0}(r-\vec{R}) \equiv W_a(r-R-\overline{r_a})$$

③ Let $g = \{\bar{g} \mid \vec{d}\} \in G$

$$\boxed{g^{-1} = \{\bar{g}^{-1} \mid -\bar{g}^{-1}\vec{d}\}}$$

$$\langle r | U_g | W_{a\vec{R}} \rangle = \langle g^{-1}\vec{r} | W_{a\vec{R}} \rangle$$

$$= W_{aR}(\bar{g}^{-1}\vec{r} - \bar{g}^{-1}\vec{d})$$

$$= W_a(\bar{g}^{-1}\vec{r} - \bar{g}^{-1}d - R - \bar{r}_a)$$

$$= W_a(g^{-1}(r - g(R + \bar{r}_a)))$$

If $\{|W_{aR}\rangle\}$ form a representation of G, this better be a sum of WFS

$$W_a\left(g^{-1}(r - g(R+\bar{r}_a))\right) \stackrel{?}{=} \sum_{R'} \sum_{b=1}^{N} B_{ba}(g, R') W_b(r - R' - \bar{r}_b)$$

a function centered at $g(R+\bar{r}_a)$

centered at $R' + \bar{r}_b$

can only be true if $R' = \underbrace{g(\widehat{R+\bar{r}_a}) - \bar{r}_b}$

$\rightarrow$ $g(R+\bar{r}_a)$ needs to be the center of a WF for all $g \in G$

$\rightarrow$ Can try to choose WFs to satisfy

$$U_g |W_{aR}\rangle = \sum_{R'} \sum_{b=1}^{N} B_{ba}(g)\, \delta_{R', \overline{g(R+\bar{r}_a) - \bar{r}_b}} |W_{bR'}\rangle$$

If this is possible, the S.G. representation

$\{ B_{ba}(g) \delta_{R', g(R+\bar{r}_a)-\bar{r}_b} \}$ is called a band representation

Assume for now we have a band representation

$g = \{E | \vec{t}\}$ $\quad U_{\vec{t}} | W_{a\vec{R}} \rangle = | W_{aR+\vec{t}} \rangle$

$$\boxed{B_{ab}(\{E|\vec{t}\}) = \delta_{ab}}$$

$$U_{g_1} U_{g_2} | W_{a\vec{R}} \rangle = \sum_{cb} B_{cb}(g_1) B_{ba}(g_2) \delta_{R', g_1 g_2 (R+\bar{r}_a)-\bar{r}_c} | W_{cR'} \rangle$$

$$U''_{g_1 g_2} |W_{a\vec{R}}\rangle = \sum_b B_{ba}(g_1 g_2)\, \delta_{R', g_1 g_2 (R + \vec{r}_a) - \vec{r}_b} |W_{bR'}\rangle$$

$$\boxed{B(g_1) B(g_2) = B(g_1 g_2)}$$

B is a representation of G

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

$$\ker B > T$$

B is a representation G_T

$\rightarrow$ B is determined by reps of $\bar{G} = G/T$

In momentum space $\rightarrow$ transformation of $|X_{ak}\rangle$

is a band representation

$$u_g|\chi_{ak}\rangle = \sum_R u_g|W_{aR}\rangle e^{ik\cdot(R+\bar{r}_a)} \qquad g=\{\bar{g}|\vec{d}\}$$

$$=\sum_b \underbrace{\sum_{RR'}}\, |W_{bR'}\rangle B_{ba}(\bar{g})\,\delta_{R',\,\underbrace{g(R+\bar{r}_a)-\bar{r}_b}}\, e^{ik\cdot(R+\bar{r}_a)}$$

$$=\sum_{bR'} |W_{bR'}\rangle B_{ba}(\bar{g})\, e^{ik\cdot(\cancel{\bar{r}_a}+[g^{-1}(R'+\bar{r}_b)-\cancel{\bar{r}_a}])}$$

$$=\sum_{bR'} |W_{bR'}\rangle B_{ba}(\bar{g})\, e^{ik\cdot(\bar{g}^{-1}(R'+\bar{r}_b)-\bar{g}^{-1}\vec{d})}$$

$$=\sum_b \underbrace{\sum_{R'} |W_{bR'}\rangle e^{i\bar{g}k\cdot(R'+\bar{r}_b)}}\left[B_{ba}(\bar{g})e^{-i\bar{g}k\cdot\vec{d}}\right]$$

$$= \sum_b |\chi_{b\bar{g}k}\rangle \underbrace{B_{ba}(\bar{g})\, e^{-i\bar{g}k\cdot\vec{d}}}_{\text{Sewing matrix for } g \text{ in tb basis}}$$

Symmetry constraint on $h^{ab}(k)$ for a band representation

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

$$= \left[\cancel{e^{i\bar{g}k\cdot\vec{d}}}\, B^{\dagger}(\bar{g})\, h(\bar{g}k)\, B(\bar{g})\, \cancel{e^{-i\bar{g}k\cdot d}}\right]^{ab}$$

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

Holds for approx th hamiltonian
as long as truncation respects symmetries