Lecture 18

Recap: $\langle \psi_{nk} | [P x_i P, P x_j P | \psi_{mk'} \rangle$

$$= \frac{(2\pi)^3}{V} \delta(\vec{k} - \vec{k}') \, i \Omega_{ij}^{nm}(k)$$

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

Berry curvature

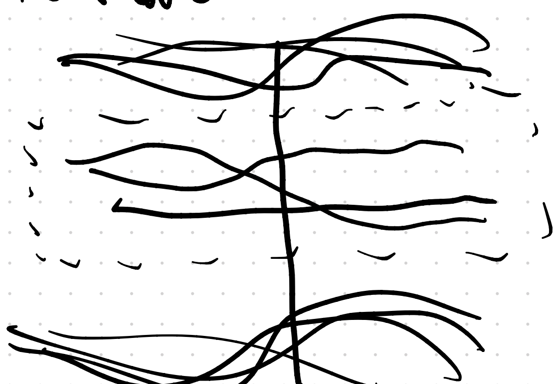
→ We have to find (Exponentially localized) Wannier functions $|W_{a\vec{R}}\rangle$ through numerical minimization in general

Useful properties $\langle W_{a\vec{R}} | W_{b\vec{R}'} \rangle = \delta_{ab} \delta_{\vec{R},\vec{R}'}$

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

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

Given a set $\{|W_{a\vec{R}}\rangle\}$ of exponentially localized WFs, what can we do



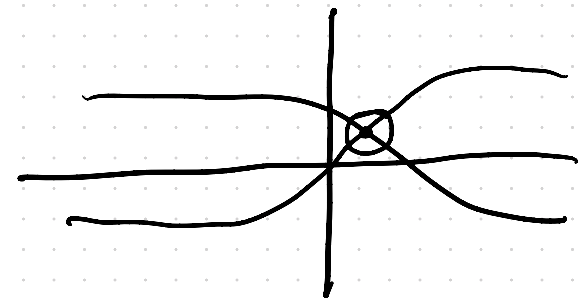
← Project onto low energy dofs → find $\{|W_{aR}\rangle\}$

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

H has discrete translation symmetry → its helpful to F.T. h

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

$$A^{nn}_{(k)} = \langle u_{nk} | \frac{\partial u_{nk}}{\partial k} \rangle$$



Tight binding basis functions

$$|\chi_{a\vec{k}}\rangle = \sum_R e^{ik\cdot(R+\bar{r}_a)} |W_{a\vec{R}}\rangle = e^{ik\cdot\bar{r}_a} |\tilde{\varphi}_{a\vec{k}}\rangle$$

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

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

$$= \left[\frac{v}{(2\pi)^3}\right]^2 \int d^3k \int d^3k' \underbrace{\langle \chi_{ak}|H|\chi_{bk'}\rangle}_{\text{Schur's lemma: } \langle \chi_{ak}|H|\chi_{bk}\rangle \left(\frac{(2\pi)^3}{v}\delta(k-k')\right)} e^{i(k\cdot(R+\bar{r}_a) - k'\cdot(R'+\bar{r}_b))}$$

$$= \frac{v}{(2\pi)^3}\int dk \left[\langle \chi_{ak}|H|\chi_{bk}\rangle e^{ik\cdot(\bar{r}_a-\bar{r}_b)}\right] e^{ik\cdot(\vec{R}-\vec{R}')}$$

$$= \frac{v}{(2\pi)^3}\int d^3k \left[e^{ik\cdot\bar{r}_a} \langle \chi_{ak} | H | \chi_{bk} \rangle e^{-ik\cdot\vec{r}_b} \right] e^{ik\cdot(R-R')}$$

$$h^{ab}(k) = \langle \chi_{ak} | H | \chi_{bk} \rangle$$ – tight binding Hamiltonian in momentum space

$$V_{ab}(k) = e^{ik\cdot\bar{r}_a}\,\delta_{ab}$$ ← "embedding matrix"

Note: $\vec{G} \in \check{T}$ in the reciprocal lattice

$$|\chi_{ak+\vec{G}}\rangle = e^{i(k+G)\cdot\bar{r}_a}\,|\tilde{\psi}_{a\vec{k}+\vec{G}}\rangle = e^{iG\cdot\bar{r}_a}\,|\chi_{a\vec{k}}\rangle$$

$$= \sum_b V_{ab}(\vec{G})\,|\chi_{b\vec{k}}\rangle$$

$$\Rightarrow \quad h^{ab}(k+\vec{G}) = \langle \chi_{ak+G} | H | \chi_{bk+G} \rangle$$

$$= \left[V^{\dagger}(G)\, h(k)\, V(G) \right]_{ab}$$

Now: Expand eigenstates of H in terms of our basis functions

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

$$P|\psi_{nk}\rangle = |\psi_{nk}\rangle \leftarrow |\psi_{nk}\rangle \in \text{low energy subspace}$$

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

u_{nk}^{a} - a vector of coefficients indexed by $a = 1, \ldots N$

$$\langle \chi_{a\vec{k}} | H | \psi_{nk} \rangle = \langle \chi_{a\vec{k}} | E_{nk} | \psi_{nk} \rangle$$

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

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

Our Schrödinger equation reduces to an $N \times N$ matrix equation

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

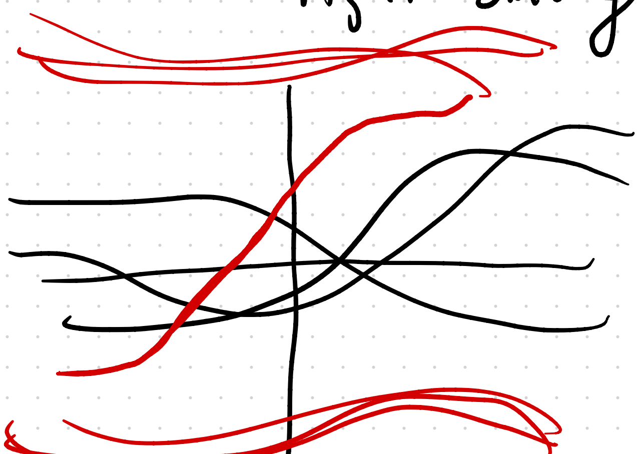
if Wannier functions are exponentially localized,

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

Pick $\Delta \sim O(\xi)$

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

Tight-binding approximation



Souza et al

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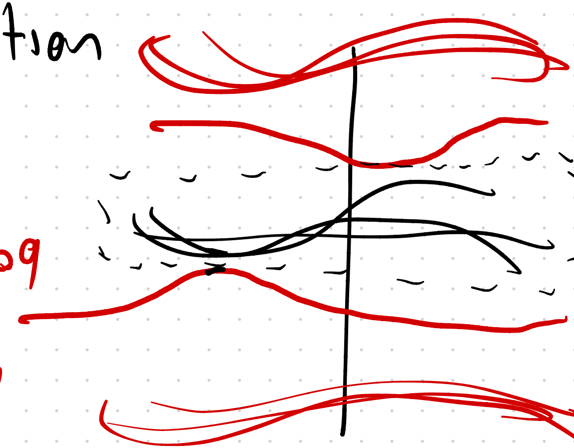
"Disentangling"



Lets return to space group Symmetries

H is invariant under a space group G $\{|\psi_{n\vec{k}}\rangle\}$ transform in representations of the space group

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

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

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

(2) $\langle r | W_{a\vec{R}} \rangle = W_{aR}(\vec{r})$ is centered at $R + \bar{r}_a$

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

(3) Let $g \in \{\bar{g} | \vec{d}\} \in G$ $\qquad g^{-1} = \{\bar{g}^{-1} | -\bar{g}^{-1}\vec{d}\}$

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

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

$\bar{r}_a = \langle W_{a0} | \vec{x} | W_{a0} \rangle$

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

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

If our Wannier fns form a representation of G

then we need

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

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

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

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

in this case, we can try to choose our Wannier fns s.t.

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

If this is possible, the representation of the space group we get is called a <u>band representation</u>

Not always possible

Assume for now we have a band representation

$B_{ab}(g)$ define the band representation

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

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

$$= U_{g_1 g_2} |W_{aR}\rangle \text{ only if}$$

$$B(g_1) B(g_2) = B(g_1 g_2)$$

$B: G \to U(N)$ and $\ker B > T$

B is a representation of G, (B is determined by representations of $\bar{G}$)

What does the band representation mean for tight-binding basis functions

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

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

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

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

$$= \sum_{b=1}^{N} |\chi_{b\bar{g}k}\rangle B_{ba}(\bar{g}) e^{-i\bar{g}k\cdot\vec{d}}$$

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

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

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

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

This holds for approximate tb hamiltonians as long as we truncate in a symmetric way