Lecture 17

Announcements:
- HW 2 solutions posted, HW2 graded
- HW 4 posted, due 10/31

① polarization density (dipole moment per unit cell)

$$P_\mu = \frac{-e|a_\mu|}{(2\pi)^3} \int d^3k \, \mathrm{tr}(A_\mu(k))$$

only well-defined modulo $e|a_\mu|$

② $\langle \psi_{nk} | [Px_\mu P, Px_\nu P] | \psi_{mk'} \rangle$

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

$$\Omega_{\mu\nu}^{nm}(\vec{k}) = \partial_\mu A_\nu^{nm} - \partial_\nu A_\mu^{nm} - i [A_\mu, A_\nu]^{nm}$$

Non-abelian Berry curvature

How do we find Wannier functions?

To find Hybrid Wannier functions:

$$\sum_n |\psi_{nk}\rangle U_{na}(k) = |\tilde{\psi}_{a k_\mu, \vec{k}_\perp}\rangle$$

we chose $U_{na}(\vec{k})$ to guarantee that $|\tilde{\psi}_{a k_\mu, \vec{k}_\perp}\rangle$ is analytic in k_μ

in our case $U_{na}(k) = W_{k_\mu \leftarrow 0} \, e^{-i\frac{\varphi_a}{2\pi}(k_\perp)}$

$$i D_\mu U = 0$$

exponentially localized in the $\vec{a}_\mu$ direction $\rightarrow$ $|W_{ank_\perp}\rangle = \frac{1}{2\pi}\int_0^{2\pi} dk_\mu \, |\Psi_{ak_\mu,\vec{k}_\perp}\rangle e^{-ink_\mu}$

To generalize: <u>if</u> we can find $N \times N$ unitary $U_{na}(\vec{k})$ s.t. $|\hat{\Psi}_{a\vec{k}}\rangle = \sum_n |\Psi_{nk}\rangle U_{na}(k)$

is analytic in $\vec{k}$ (all components)

then $|W_{aR}\rangle = \frac{V}{(2\pi)^3}\int d^3k \, |\hat{\Psi}_{ak}\rangle e^{-i\vec{k}\cdot R}$

would be localized exponentially in <u>all</u> directions

$|W_{aR}\rangle$ - Wannier functions

Centers of Wannier functions:

$$\langle \vec{r}_a \rangle = \langle W_{aR} | \vec{x} | W_{aR} \rangle = \left(\frac{v}{(2\pi)^3}\right) \int d^3k \, d^3k' \langle \tilde{\Psi}_{ak} | \vec{x} | \tilde{\Psi}_{ak'} \rangle e^{iR(k-k')}$$

$$= \left(\frac{v}{(2\pi)^3}\right)^2 \int d^3k \, d^3k' \, e^{iR\cdot(k-k')} \left(i \frac{\partial}{\partial k} \delta(k-k') + \tilde{A}_{aa}(\vec{k}) \delta(\vec{k}-\vec{k}') \right)$$

$$= \vec{R} + \frac{v}{(2\pi)^3} \int d^3k \, \tilde{\vec{A}}_{aa}(\vec{k})$$

$$\tilde{A}_{ab}(k) = i \langle \tilde{u}_{ak} | \frac{\partial \tilde{u}_{bk}}{\partial k_\mu} \rangle$$

Note: $\frac{v}{(2\pi)^3}\int d^3k \, \vec{A}_{aa}(\vec{k}) \neq \frac{\varphi}{2\pi}$

diagonal element of a matrix

non-abelian Berry phase eigenvalue of Wilson loop.

$$\boxed{\text{Wannier function centers do not coincide in general with Hybrid Wannier Function centers}}$$

$\langle \vec{r}_a \rangle$ is not gauge invariant

If we want something gauge invariant:

- Hybrid Wannier function centers

- $$\sum_a \langle \vec{r}_a \rangle = N\vec{R} + \frac{V}{(2\pi)^3} \int d^3k \, \mathrm{tr}(\vec{A})$$

is gauge invariant modulo lattice vectors $\vec{R}$

(electronic contribution to) dipole moment per unit cell

Big picture summary of finding Wannier functions:

$$|\tilde{\psi}_{a\vec{k}}\rangle = \sum_n |\psi_{nk}\rangle U_{na}(k)$$

$$\updownarrow$$

$$|W_{aR}\rangle[U_{na}(k)] = \frac{v}{(2\pi)^3}\int d^3k\, |\tilde{\psi}_{a\vec{k}}\rangle e^{-iR\cdot\vec{k}}$$

$$G[U_{na}(k)] = \sum_{a=1}^{N} \langle W_{a\vec{R}}|x^2|W_{aR}\rangle - |\langle W_{aR}|\vec{x}|W_{aR}\rangle|^2$$

$\downarrow$ numerical minimization

optimal U

Caveats:

1. Not guaranteed to give us something exponentially localized

2. Does not enforce symmetry

For space group symmetries $g = \{h|\vec{d}\}$

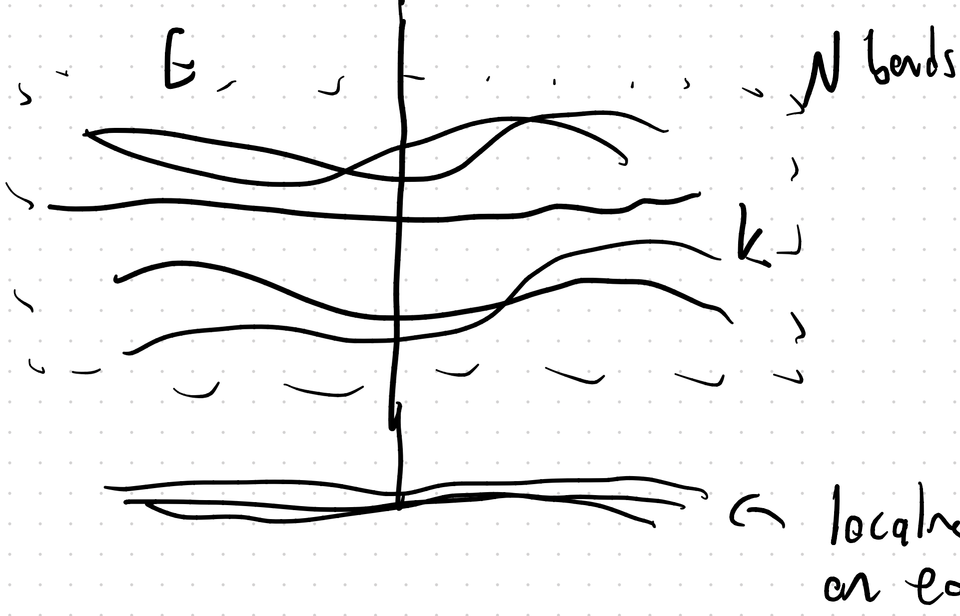
$$U_g|\psi_{nk}\rangle = \sum_m |\psi_{m\,hk}\rangle B_k^{mn}(g)$$

For our $N \times N$ unitary matrices $U(\vec{k})$

we need $U(hk) = B_k^\dagger(g)\, U(k)\, B_k(g)$

Two main uses (for us) for Wannier functions

1. Wannier fns help us reduce the dimensionality of the Schrödinger equation



If we have Wannier fns for the bands in the dashed box, we can truncate our Hamiltonian

$$\left\{ |W_{aR}\rangle \,,\; a = 1 \ldots N \right\}$$

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

exponentially localised Wannier functions

$$\| h^{ab}(R-R') \| \to 0 \text{ exponentially}$$

tight-binding approx: set $h^{ab}(R-R') = 0$

if $|R-R'| > \Delta$

(2) Try to prove whether or not exponentially localised Wannier fns exist for a given set of bands

→ topological insulators

Start w/ 1

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

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

Introduce tight-binding basis functions

$$|\chi_{a\vec{k}}\rangle = \sum_{R} e^{i\vec{k}\cdot(\vec{R}+\langle\vec{r}_a\rangle)} |W_{a\vec{R}}\rangle$$

$$\Rightarrow |W_{a\vec{R}}\rangle = \frac{v}{(2\pi)^3}\int d^3k\, e^{-i\vec{k}(R+\langle r_a\rangle)} |\chi_{ak}\rangle$$

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

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

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

$$= \frac{v}{(2\pi)^3}\int d^3k\, h^{ab}(k) e^{ik(R-R'+\langle r_a\rangle - \langle r_b\rangle)}$$

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

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

column vector of expansion coefficients

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

$$\sum_{ab} |\chi_{ak}\rangle\langle\chi_{ak}|H|\chi_{bk}\rangle u^b_{nk} = \sum_a E_{nk} u^a_{nk} |\chi_{ak}\rangle$$

$|\psi_{nk}\rangle$ is an eigenstate of H if

$$\boxed{\sum_b h^{ab}(k)\, u^b_{nk}(k) = E_{nk}\, u^a_{nk}}$$

$N \times N$
matrix

Approximations: $h^{ab}(R-R') \to 0$ when R, R'
are far apart

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

approximate tight-binding Hamiltonian

$$\lfloor h^{ab}(R-R')\rfloor = \frac{v}{(2\pi)^3}\int d^3k \ \ \tilde{h}^{ab}(k) \ \ e^{ik\cdot(R-R'+\langle r_a\rangle-\langle r_b\rangle)}$$

Summary: $|W_{aR}\rangle$ wannier functions

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

tight-binding Hamiltonian $\lfloor h^{ab}(R-R')\rfloor = \frac{v}{(2\pi)^3}\int d^3k \ \ \tilde{h}^{ab}(k) \ \ e^{ik\cdot(R-R'+\langle r_a\rangle-\langle r_b\rangle)}$