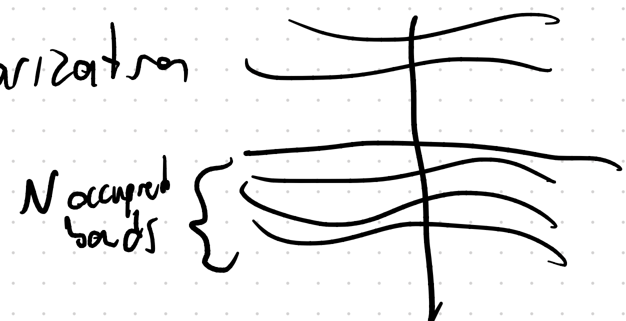
Lecture 17

Announcements: Final presentation suggested topics will be posted after class

- Email me your choice by 11/12
- Presentation logistics: 12/3, 12/5, 12/10

  20 min + 5 mins questions

Recap: Hybrid Wannier fns and polarization



dipole moment per unit volume

$$\vec{P} = \frac{Ne}{v}\vec{X}_0 - \frac{e}{(2\pi)^3}\int d^3k \, tr(\vec{A}(k))$$

ionic center of charge in the unit cell

$$= \frac{1}{v}\left(Ne\vec{X}_0 - e\sum_{a=1}^{N}\int d^2k_\perp \, \vec{t}_i \, \varphi_i^a(k_\perp)\right)$$

$e^{i\varphi_i^a(k_\perp)}$ – eigenvalues of the Wilson loop in the i-direction

$\vec{P}$ only well-defined modulo $\frac{e\vec{t}}{v}$ for $\vec{t} \in T$

Can we extend this logic → get functions exponentially localized in all 3 directions

simultaneously diagonalize Px_iP and Px_jP

We can only do this if $[Px_iP, Px_jP] = 0$

Take our wavepacket state

$$|f\rangle = \sum_{a=1}^{N} \frac{V}{(2\pi)^3} \int d^3k \, |\psi_{ak}\rangle f_{a\vec{k}}$$

$$[Px_iP, Px_jP]|f\rangle = ?$$

$$P x_i P |f\rangle = \sum_{a=1}^{N} \frac{v}{(2\pi)^3} \int d^3k \, |\psi_{a\vec{k}}\rangle [i D_i f]_{a\vec{k}}$$

$$[D_i f]_{a\vec{k}} = \left(\frac{\partial f_{a\vec{k}}}{\partial k_i} - i \sum_{b=1}^{N} A_i^{ab}(\vec{k}) f_{b\vec{k}} \right)$$

$$[P x_i P, P x_j P] |f\rangle = \sum_{a=1}^{N} \frac{v}{(2\pi)^3} \int d^3k \, |\psi_{a\vec{k}}\rangle \left[i D_i [i D_j f] - i D_j [i D_i f] \right]_{a\vec{k}}$$

$$= -\sum_{a=1}^{N} \frac{v}{(2\pi)^3} \int d^3k \, |\psi_{a\vec{k}}\rangle \left[D_i D_j f - D_j D_i f \right]_{a\vec{k}}$$

$$D_i D_j f = \left(\frac{\partial}{\partial k_i} - i A_i \right) \left(\frac{\partial}{\partial k_j} - i A_j \right) f$$

$$= \frac{\partial^2 f}{\partial k_i \partial k_j} - i A_i \frac{\partial f}{\partial k_j} - \frac{\partial}{\partial k_i} (A_j f) - A_i A_j f$$

$$D_iD_jf - D_jD_if = \cancel{\frac{\partial^2 f}{\partial k_i \partial k_j}} - iA_i \frac{\partial f}{\partial k_j} - \frac{\partial}{\partial k_i}(A_j f) - A_iA_j f$$

$$-\left[\cancel{\frac{\partial^2 f}{\partial k_i \partial k_j}} - iA_j \frac{\partial f}{\partial k_i} - \frac{\partial}{\partial k_j}(A_i f) - A_jA_i f\right)$$

$$= -i\left[\frac{\partial A_j}{\partial k_i} - \frac{\partial A_i}{\partial k_j} - i[A_i, A_j]\right] f$$

$$\equiv -i\sum_{b=1}^{N}\Omega_{ij}^{ab} f_{b\vec{k}}$$

(non-abelian)

$$\Omega_{ij}^{(\vec{k})} = \frac{\partial A_i}{\partial k_j} - \frac{\partial A_j}{\partial k_i} - i[A_i, A_j]$$ - Berry curvature

→ The Berry curvature $\Omega_{ij}(k)$ tells us by how much projected position operators fail to commute

$$[Px_iP, Px_jP]|f\rangle = \frac{v}{(2\pi)^3}\int d^3k\, |\psi_{ak}\rangle \sum_{b=1}^{N} \Omega_{ij}^{ab}(k) f_{b\vec{k}}$$

unless $\Omega_{ij}(k) = 0$ for all $\vec{k}$, we can't diagonalize Px_iP and Px_jP.

Recall that for Hybrid Wannier fns

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

$$e^{-ik\cdot x} H e^{ik\cdot x}|u_{nk}\rangle = E_{nk}|u_{nk}\rangle$$

$$\sum_{n=1}^{N} |\psi_{nk}\rangle U_{na}(k) \equiv |\tilde{\psi}_{a,k_i,\vec{k}_\perp}\rangle$$

choose $U_{na}(k)$ s.t. $|\tilde{\psi}_{a,k_i,k_\perp}\rangle$ was an analytic fn of k_i

$$U(k) = W_{k_i \leftarrow k_0}(k_\perp)\, e^{-i\frac{\varphi_a(k_\perp)}{2\pi}}\, \vec{g}_a$$

$$H(k)\,|u_{nk}\rangle = E_{nk}\,|u_{nk}\rangle$$

Electric field $H(k - E_0 t)$

$$|W_{ank_\perp}\rangle = \frac{1}{2\pi}\int_0^{2\pi} dk_i\, |\tilde{\psi}_{a,k_i,\vec{k}_\perp}\rangle\, e^{-ink_i}$$

To generalize: look for $N \times N$ periodic unitary

$U_{na}(k)$ s.t.

$$|\tilde{\psi}_{ak}\rangle = \sum_{n=1}^{N} |\psi_{nk}\rangle U_{na}(k)$$ is analytic as a fn of every component of $\vec{k}$

$$U_{\vec{t}}|\tilde{\psi}_{ak}\rangle = e^{-ik\cdot t}|\tilde{\psi}_{ak}\rangle$$

<u>If</u> we can do this, then

$$|W_{a\vec{R}}\rangle = \frac{V}{(2\pi)^3}\int d^3k\, |\tilde{\psi}_{ak}\rangle e^{-i\vec{k}\cdot\vec{R}}$$ will be exponentially localized

Wannier function

$$\langle r|W_{a\vec{R}}\rangle = W_{a\vec{R}}(r) \xrightarrow[r\to\infty]{} e^{-|r-R|/\xi}$$

Important properties

$$\langle W_{a\vec{R}} | W_{b\vec{R}'} \rangle = \left[\frac{v}{(2\pi)^3}\right]^2 \int d^3k\, d^3k' \langle \tilde{\Psi}_{ak} | \tilde{\Psi}_{bk'} \rangle e^{+i(k\cdot R - k'\cdot R')}$$

$$= \delta_{ab} \frac{v}{(2\pi)^3} \int d^3k\, e^{ik\cdot(R-R')}$$

$$= \delta_{ab}\, \delta_{R,R'}$$

under Bravais lattice translations:

$$U_{\vec{t}} | W_{aR} \rangle = \frac{v}{(2\pi)^3} \int d^3k\, U_t | \tilde{\Psi}_{ak} \rangle e^{-ik\cdot R}$$

$$= \frac{v}{(2\pi)^3} \int d^3k\, | \tilde{\Psi}_{ak} \rangle e^{-ik\cdot(R+\vec{t})} = | W_{a\,\vec{R}+\vec{t}} \rangle$$

Big picture of How we find Wannier functions

$$H \to \{|\psi_{nk}\rangle\}_{n=1}^{N} \qquad U_{na}(k) \text{ - } N\times N \text{ unitary matrix}$$

$$|W_{a\vec{R}}[U]\rangle = \frac{V}{(2\pi)^3}\int d^3k \sum_{n=1}^{N} |\psi_{nk}\rangle U_{na}(k) e^{-ik\cdot\vec{R}}$$

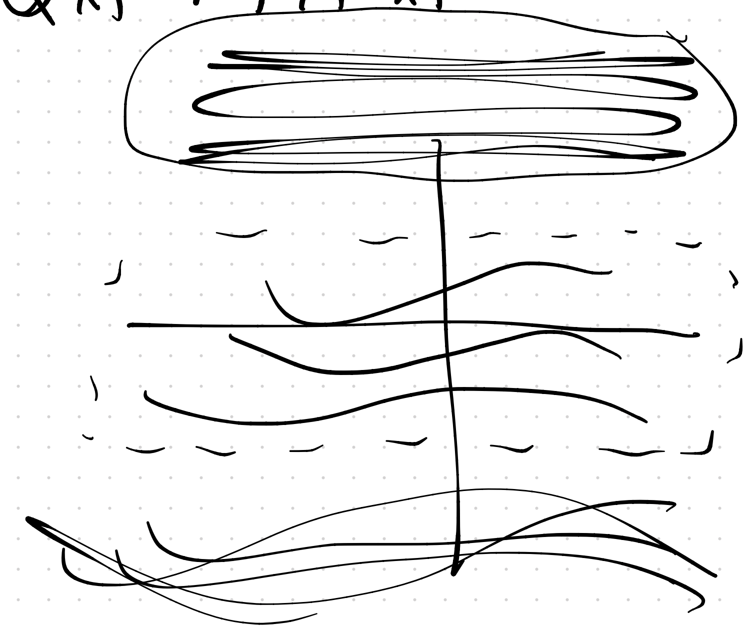
Metric for localization

$$G[U] = \sum_{a=1}^{N} \langle W_{a0}[U]|\, x^2 |W_{a0}[U]\rangle - |\langle W_{a0}[U]|\vec{x}\,|W_{a0}[U]\rangle|^2$$

discretize BZ → numerically minimize G as a functional of U → maximally localized Wannier functions

Marzari et al Rev Mod Phys

$$Px^2P = PxQxP + PxPxP$$



core ~~b~~ands

Caveats: ① Numerical minimization might not converge, might not give us something exponentially localized

② If we want WFs that respect the symmetries of a space group, we need to modify this procedure

It is not always the case that a given set of bands has exponentially localized, symmetric Wannier Functions

③ Wannier centers $\langle W_{aR} | \vec{x} | W_{aR} \rangle$

$$= \left(\frac{v}{(2\pi)^3}\right)^2 \int d^3k\, d^3k' \langle \Psi_{ak} | \vec{x} | \Psi_{ak'} \rangle e^{iR(k-k')}$$

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

$$= \vec{R} + \frac{v}{(2\pi)^3} \int d^3k\, \tilde{A}_{aa}(k) \qquad \tilde{A}_{ab}(k) = i \left\langle \tilde{u}_{ak} \middle| \frac{\partial \tilde{u}_b}{\partial \vec{k}} \right\rangle$$

diagonal aa matrix element of $\tilde{A}$ - not an eigenvalue $\frac{\varphi_a}{2\pi}$

→ Wannier centers are not gauge invariant

$$\sum_{a=1}^{N} \langle W_{aR} | \vec{x} | W_{a\vec{R}} \rangle = N\vec{R} + \frac{V}{(2\pi)^3}\int d^3k \; \mathrm{tr}\, \tilde{A}(k)$$

electronic contribution to $\vec{P}$

Two main uses for Wannier functions

1. WFs reduce the dimensionality of Schrödinger Eqn

N states of interest $\rightarrow |W_{aR}\rangle$

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

2. In proving whether or not exponentially localized WFs exist, we will discover topological insulators