Lecture 17

Announcements: HW 3 is due Thursday

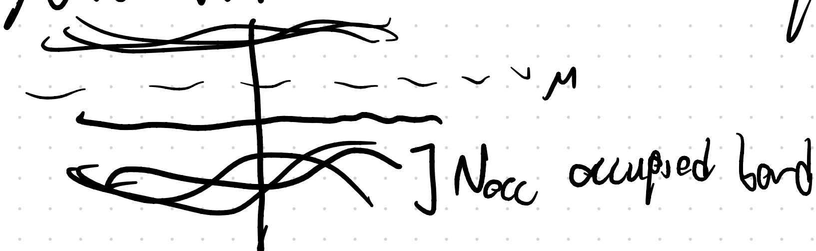
- Final presentations: topic ideas will be posted today

Email me your topic choice by 4/8

Presentations 4/29, 5/1, 5/6

20 min + 5 mins for questions

Recap: Hybrid Wannier Functions and polarization in insulators



electric dipole moment per unit volume

$$\vec{P}_v = \frac{N_{occ}\, e}{v} \vec{x}_0 - \frac{e}{(2\pi)^3} \int d^3k \, \mathrm{tr}(\vec{A}(k))$$

Berry connection

ionic center of charge in the unit cell

$$= \frac{1}{v} \left(N e \vec{x}_0 - e \sum_{i=1}^{3} \sum_{a=1}^{N_{occ}} \int d^2k_\perp \, \vec{t}_i \, \varphi_i^a(k_\perp) \right)$$

$e^{i\varphi_i^a(k_\perp)}$ — Wilson loop eigenvalues $\leftarrow$ centers of Hybrid Wannier functions

$\vec{P}_v$ is only well-defined modulo $\frac{e}{v}\vec{t}$ for $\vec{t} \in T$ the Bravais lattice

Hybrid Wannier Functions: localized in t_i direction, and extended in $t_{j \neq i}$

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

HWFs: PX_iP eigenstates

→ Simultaneously diagonalize PX_iP and PX_jP

We can only do this if $[PX_iP, PX_jP] = 0$

Take a wavepacket $|F\rangle = \frac{V}{(2\pi)^3} \int d^3k \sum_{a=1}^{N_{occ}} |\psi_{ak}\rangle f_{a\vec{k}}$

$$[Px_iP, Px_jP]|f\rangle \stackrel{?}{=} 0 \; ?$$

$$Px_iP|f\rangle = \frac{V}{(2\pi)^3}\int d^3k \sum_{a=1}^{N_{occ}} |\psi_{ak}\rangle [iD_i f]_{a\vec{k}}$$

$$[D_i f]_{ak} = \frac{\partial f_{ak}}{\partial k_i} - i\sum_{b=1}^{N_{occ}} A_i^{ab} f_{bk}$$

$$[Px_iP, Px_jP]|f\rangle = \sum_{a=1}^{N_{oq}} \frac{V}{(2\pi)^3}\int d^3k \, |\psi_{ak}\rangle \left[iD_i(iD_j f) - iD_j(D_i f)\right]_{ak}$$

$$= -\sum_{a=1}^{N_{occ}} \frac{V}{(2\pi)^3}\int d^3k \, |\psi_{ak}\rangle [D_iD_j f - D_jD_i f]_{a\vec{k}}$$

$$D_iD_j f = \left(\frac{\partial}{\partial k_i} - iA_i\right)\left(\frac{\partial}{\partial k_j} - iA_j\right)\vec{f}$$

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

$$D_i D_j f - D_j D_i f = \left(\cancel{\frac{\partial^2 \vec{f}}{\partial k_i \partial k_j}} - iA_i \frac{\partial \vec{f}}{\partial k_j} - i\frac{\partial}{\partial k_i}(A_j \vec{f}) - A_i A_j \vec{f} \right)$$

$$- \left(\cancel{\frac{\partial^2 \vec{f}}{\partial k_j \partial k_i}} - iA_j \frac{\partial \vec{f}}{\partial k_i} - i\frac{\partial}{\partial k_j}(A_i \vec{f}) - A_j A_i \vec{f} \right)$$

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

$$= -i \sum_{b=1}^{N_{occ}} \Omega_{ij}^{ab}(k) f_{b\vec{k}}$$

$$\Omega_{ij} = \frac{\partial A_i}{\partial k_j} - \frac{\partial A_j}{\partial k_i} - i[A_i, A_j]$$ ← (non-abelian) Berry Curvature

$$\langle \psi_{a\vec{k}} | [P x_i P, P x_j P] | \psi_{b\vec{k}'} \rangle = -i\, \Omega^{ab}_{ij}(\vec{k})\, \delta(k-k')$$ [illegible]

The Berry curvature tells us by how much the projected position operators fail to commute

Cannot simultaneously diagonalize $P x_i P$, $P x_j P$ unless

$$\Omega_{ij}(\vec{k}) = 0 \text{ for all } \vec{k}$$

Berry Curvature and change of basis

$$A_i(k) \rightarrow U^\dagger(k) A_i U + i U^\dagger \frac{\partial U}{\partial k_i}$$

$$\Omega_{ij} \equiv \frac{\partial}{\partial k_i} A_j - \frac{\partial A_i}{\partial k_j} - i\left[A_i, A_j\right]$$

$$\rightarrow \frac{\partial}{\partial k_i}\left[U^\dagger A_j U + i U^\dagger \frac{\partial U}{\partial k_j}\right] - \frac{\partial}{\partial k_j}\left[U^\dagger A_i U + i U^\dagger \frac{\partial U}{\partial k_i}\right]$$

$$- i\left[U^\dagger A_i U + i U^\dagger \frac{\partial U}{\partial k_i}, U^\dagger A_j U + U^\dagger \frac{\partial U}{\partial k_j}\right]$$

$$= U^\dagger(k) \Omega_{ij} U(k)$$

We need a different approach to find Wannier functions

For HWF, diagonalizing $P x_j P$ was a shortcut to finding

$$|\tilde{\psi}_{bk}\rangle = \sum_{n=1}^{N_{occ}} |\psi_{ak}\rangle U_{ab}(k) = |\tilde{\psi}_{b,k_j,k_\perp}\rangle$$

choose $U_{an}(\vec{k})$ $|\tilde{\psi}_{a,k_j,k_\perp}\rangle$ was an analytic function of k_j

$$U(k) = W_{k_j \leftarrow k_0}(k_\perp) e^{-i \varphi_a(k_\perp) \frac{\varsigma_a}{2\pi}}$$

$$|W_{a n k_\perp}\rangle = \frac{1}{2\pi} \int_0^{2\pi} dk_j \, |\tilde{\psi}_{a,k_j,k_\perp}\rangle e^{-i n k_j}$$

To generalise: look for $N_{occ} \times N_{occ}$ unitary matrices periodic in $\vec{k}$ s.t.

$$|\tilde{\psi}_{ak}\rangle = \sum_{b=1}^{N_{occ}} |\psi_{bk}\rangle U_{ba}(k)$$ is analytic in all components of $\vec{k}$

If we can do this then

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

Wannier function

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

Important properties:

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

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

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

$$= \delta_{ab} \delta_{RR'}$$

under Bravais lattice translations

$$u_t |W_{aR}\rangle = \frac{v}{(2\pi)^3}\int d^3k \; u_t |\tilde{\psi}_{ak}\rangle e^{-ik\cdot R}$$

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

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

Big Picture for Finding Wannier Functions

$$H \longrightarrow \{|\psi_{nk}\rangle\}_{n=1}^{N_{occ}} \quad \text{obtained by diagonalization}$$

$$|W_{aR}[U]\rangle = \frac{v}{(2\pi)^3}\int d^3k \sum_{n=1}^{N_{occ}} |\psi_{nk}\rangle U_{na}(k) e^{-i\vec{k}\cdot\vec{R}}$$

$U_{na}(k)$ is an $N_{occ} \times N_{occ}$ matrix

Metric for localization

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

Numerical minimization $\rightarrow$ find U_* to minimize G

$\rightarrow |W_{aR}[U_*]\rangle$ maximally localized Wannier functions

Marzari et al Rev. Mod. Phys

Caveats: 1) Numerical minimization might not converge.

Even if it converges $|W_{aR}[U^*]\rangle$ might not be exponentially localized

(2) This procedure needs to be modified if we want $|W_{a\ell}[U^{\dagger}]\rangle$ to transform in a representation of the space group

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

Wannier centers $\langle W_{a\vec{R}} | \vec{x} | W_{a\vec{R}} \rangle$

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

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

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

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

$$= \left[U^{\dagger} A U + i U^{\dagger} \frac{\partial U}{\partial k} \right]_{aa}$$

diagonal matrix element of $\tilde{A}$ NOT an observable

→ Wannier centers are not gauge invariant

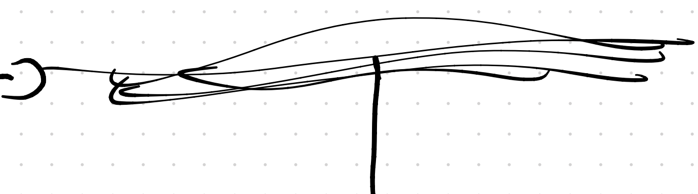
$$\sum_{a=1}^{N_{occ}} \langle W_{aR} | \vec{x} | W_{aR} \rangle = N_{occ} R + \frac{V}{(2\pi)^3} \int d^3k \, \mathrm{tr}\left(\tilde{A}_{an}(k)\right)$$

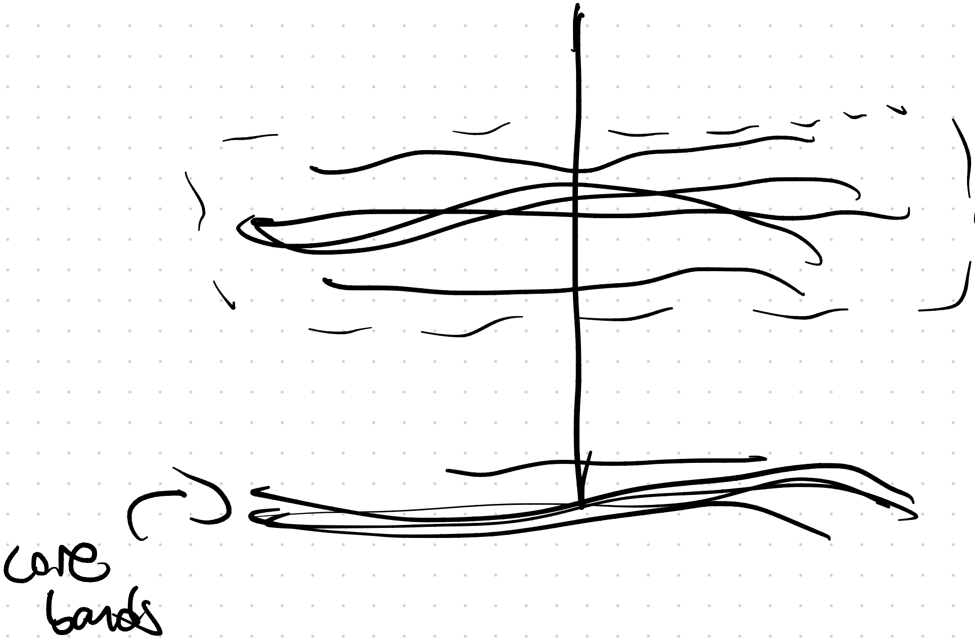
electronic contribution to $\vec{P}_V$

Two main uses for Wannier functions (WFs)

① WFs reduce dimensionality of the Schrödinger equation

scattering states





$\leftarrow N$ interesting states $\rightarrow |w_{aR}\rangle$

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

② The existence or lack thereof of WF will allow us to define topological insulators