Lecture 18

Announcements:
- HW 3 due today
- HW 4 will be posted tonight, due 11/6
- HW 2 Solutions posted

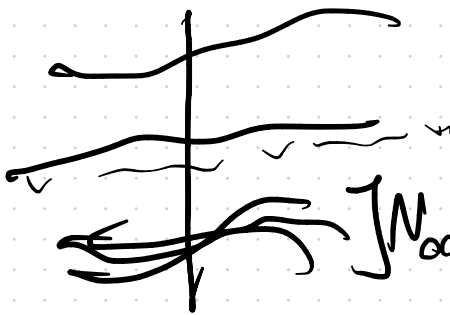
Final presentations:
- topic ideas posted

Email me your topic choice by 11/11

Presentations will be on 12/2, 12/4, 12/9

~20 mins / presentation

Recap: Hybrid Wannier Functions, polarization / dipolemoment



electric dipole moment per unit cell

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

$\vec{X}_0$: center of ionic charge in the unit cell

$\vec{p}$ is only well-defined modulo $e\vec{t}$ for $\vec{t} \in T$

Hybrid Wannier functions → localized in one direction

Can we find functions localized in all 3 directions?

HWFs: diagonalizing Px_iP

Simultaneously diagonalize Px_iP and Px_jP

only possible if $[Px_iP, Px_jP] = 0$

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

$$P x_i P |f\rangle = \frac{V}{(2\pi)^3}\int d^3k \sum_{a=1}^{N_{occ}} |\psi_{ak}\rangle \left[i D_i f \right]_{ak}$$

$$\left[D_i f \right]_{ak} = \frac{\partial f_{ak}}{\partial k_j} - i \sum_{b=1}^{N_{occ}} A_j^{ab}(k)\, f_{b\vec{k}}$$

$$= \left(\frac{\partial \vec{f}_k}{\partial k_i} - i A_i(k) \vec{f}_k \right)_a$$

$$\left[P x_i P, P x_j P \right] |f\rangle = \sum_{a=1}^{N_{occ}} \int d^3k \frac{V}{(2\pi)^3} |\psi_{ak}\rangle \left(D_i(D_j f) - D_j(D_i f) \right) \Big]$$

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

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

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

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

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

$$= -i \sum_{b=1}^{N_{occ}} \Omega^{ab}_{ij}(k) f_{bk}$$

$$\Omega_{ij} = \frac{\partial A_j}{\partial k_j} - \frac{\partial A_j}{\partial k_i} - i[A_i, A_j] \leftarrow \text{Berry curvature}$$

$$\langle \psi_{ak} | [P x_i P, P x_j P] | \psi_{bk'} \rangle = -i\, \Omega^{ab}_{ij}(k) \left[\frac{(2\pi)^3}{V} \delta(k-k')\right]$$

The Berry curvature measures by how much Px_iP and Px_jP fail to commute

$\rightarrow$ we can only simultaneously diagonalize Px_iP and Px_jP when $\Omega_{ij}(k) = 0$

Berry curvature and change of basis:

$$A_i(k) \rightarrow U^{\dagger} A_i U + i U^{\dagger} \frac{\partial U}{\partial k_i} = A' \quad U(k) \text{ is unitary } N_{occ} \times N_{occ}$$

$$\Omega'_{ij} = \frac{\partial}{\partial k_i} A'_j - \frac{\partial}{\partial k_j} A'_i - i[A'_i, A'_j]$$

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

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

$$= U^\dagger \Omega_{ij}(k) U$$ ← trace, eigenvalues of Ω_{ij} are gauge invariant, observable

$\Rightarrow$ $[Px_iP, Px_jP] \neq 0$ in one basis,

it's nonzero in every basis

We need a different approach to find localized functions

For hybrid WFs $|\tilde{\psi}_{bk}\rangle = \sum_{a=1}^{N_{occ}} |\psi_{ak}\rangle U_{ab}(k) = |\tilde{\psi}_{bk_j,\vec{k}_\perp}\rangle$

choosing U from diagonalizing Px_jP gave $|\tilde{\psi}_{bk_j,\vec{k}_\perp}\rangle$ that is smooth in k_j

$$\Rightarrow \quad |W_{an k_\perp}\rangle = \frac{1}{2\pi}\int_0^{2\pi} dk_j \, |\tilde{\Psi}_{a k_j, k_\perp}\rangle e^{-ink_j}$$

To generalize: look for $N_{occ} \times N_{occ}$ unitary matrix $U(k)$ s.t.

$$|\tilde{\Psi}_{ak}\rangle = \sum_{b=1}^{N_{occ}} |\Psi_{bk}\rangle U_{ba}(k)$$ smooth in all components of $\vec{k}$

If we can find U then

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

Wannier Function

Big picture for finding Wannier Functions (WFs)

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

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

Metric for localization

$$G[U] = \sum_{a=1}^{N_{occ}} \langle w_{a\vec{0}}[U] | \vec{x}\cdot\vec{x} | w_{a\vec{0}}[U] \rangle - |\langle w_{a0}[U] | \vec{x} | w_{a0}[U] \rangle|^2$$

Numerical minimization → find U_* that minimizes G ← Marzari et al Rev. Mod. Phys.

Caveats ① Numerical minimization might not converge

② Even if it does converge, $|w_{a0}[U]\rangle$ might

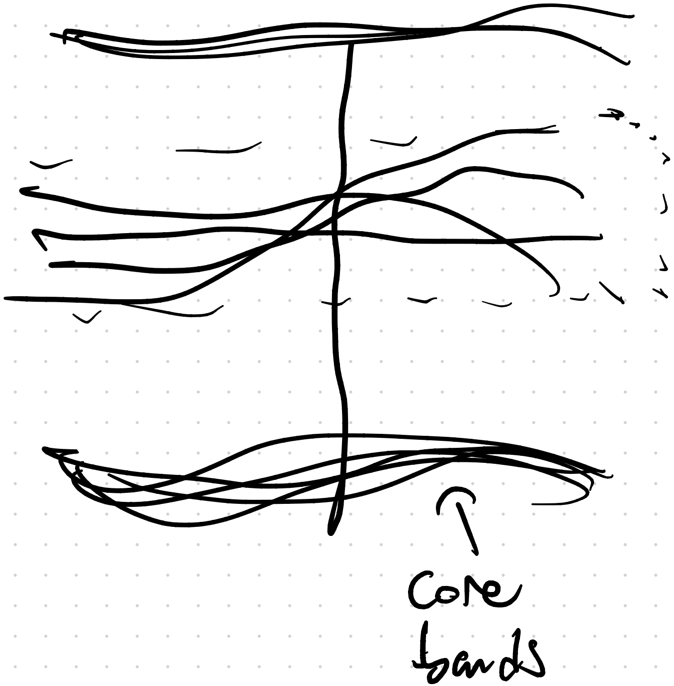
→ not be exponentially localized

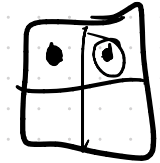
③ The naive procedure doesn't know about space group symmetries

Not always possible

Two main uses for Wannier functions

① WFs reduce the dimensionality of the Schrodinger equations





~N interesting states → $|W_{a\vec{R}}\rangle$

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

(2) The existence or lack thereof of WF to define topological insulators

Lets say we have wannier functions $|W_{a\vec{R}}\rangle$

Important properties:

$$\langle W_{aR}|W_{bR'}\rangle = \left(\frac{V}{(2\pi)^3}\right)^2 \int d^3k\, d^3k' \langle \psi_{ak}|\psi_{bk'}\rangle e^{i(k\cdot R - k'\cdot R')}$$

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

$$= \delta_{ab}\, \delta_{RR'} \qquad \text{orthonormal}$$

Under Bravais lattice translations

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

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

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

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

$$= \left(\frac{v}{(2\pi)^3}\right)^2 \int dk\, dk' \langle \tilde{\Psi}_{ak}|\vec{x}|\tilde{\Psi}_{bk'}\rangle e^{iR\cdot(k-k')}$$

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

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

diagonal matrix element
<u>NOT</u> an eigenvalue

Centers of WFs are basis dependent