Compressed Modes for Topological Insulators using Manifold Projection

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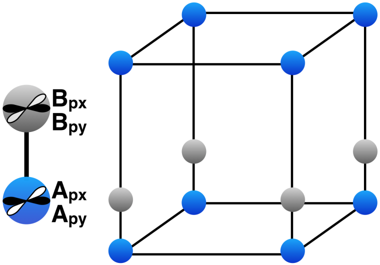
Overview

1. Introduce Fu's topological crystalline insulator model.
2. Calculate compressed Wannier modes.
3. Use compressed Wannier modes in topological analysis.
4. Suggest a new form of compressed Wannier modes based on manifold projection.

Fu's Model

Liang Fu. Phys. Rev. Lett. 106,106802, (2011)

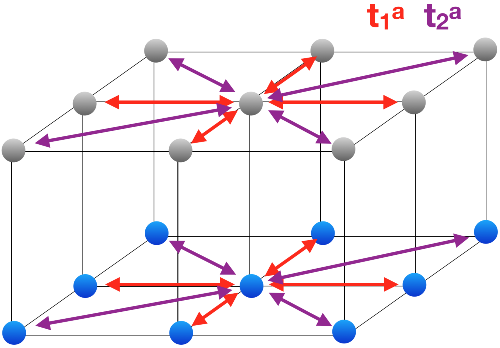
- Topological crystalline insulator.
- Z_2 classification:
  - $\rightarrow$ $(\hat{C}_4\hat{K})^2 = -1$ allows doubly degenerate states.
- Tetragonal lattice:



Real-Space Tight-Binding Hamiltonian

$$H(\mathbf{r}) = \sum_n H_n^A + H_n^B + H_n^{AB}$$

- Full Intralayer Hamiltonian term:
  $H_n^a = \sum_{i,j} t^a(\mathbf{r}_i - \mathbf{r}_j) \sum_{\alpha,\beta} c^\dagger_{a\alpha}(\mathbf{r}_i, n) e^{ij}_\alpha e^{ij}_\beta c_{a\beta}(\mathbf{r}_j, n)$

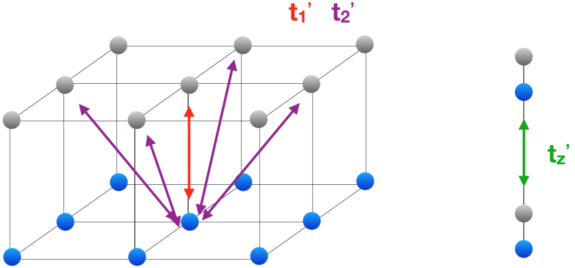


Real-Space Tight-Binding Hamiltonian

$$H(\mathbf{r}) = \sum_n H_n^A + H_n^B + H_n^{AB}$$

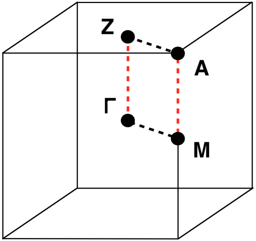
- Full Interlayer Hamiltonian term:

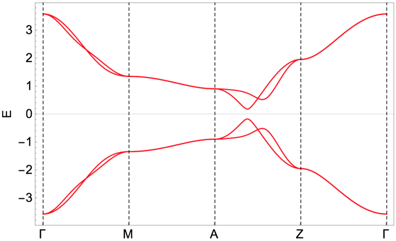
$$H_n^{AB} = \sum_{i,j} t^{'}(\mathbf{r}_i - \mathbf{r}_j)\Big[\sum_{\alpha} c^{\dagger}_{A\alpha}(\mathbf{r}_i, n) c_{B\alpha}(\mathbf{r}_j, n) + \mathrm{H.c.}\Big] +$$
$$t_z^{'} \sum_i \sum_j \left[c^{\dagger}_{A\alpha}(\mathbf{r}_i, n) c_{B\alpha}(\mathbf{r}_i, n+1) + \mathrm{H.c.}\right]$$



Band Structure

- Bulk insulator.

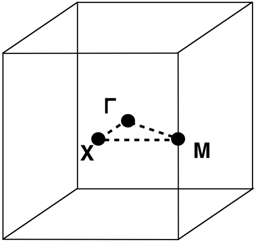


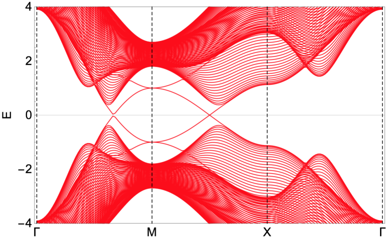


- $\hat{C}_4\hat{K}$ respected symmetry:
  - → High symmetry axis' MA and ΓZ.
  - → High symmetry points Γ, M, A, and Z; Where doubly degenerate states occur.

Band Structure

- Surface states exposed by slab band structure.
  - → Broken periodic boundary conditions in $\mathbf{k_z}$ direction.





- How can we investigate this non-trivial system in real-space?

Compressed Wannier Modes

Vidvuds Ozoliņš, et al. PNAS U.S.A. 110, 18368–18373 (2013)

- A variational approach for finding Wannier functions.
- Minimizing the L_1-norm produces localized real-space functions with compact support.

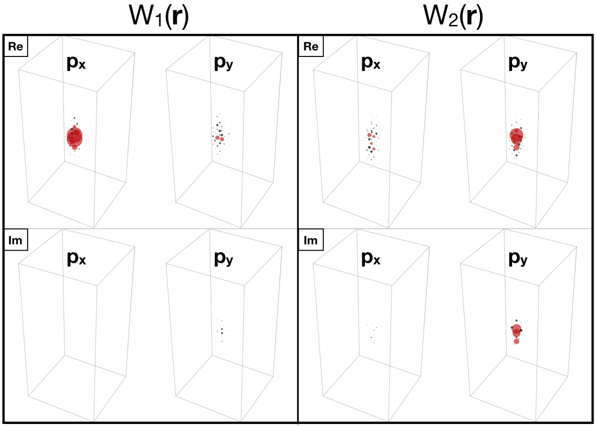
$$E_{\min} = \min_{W} \sum_{j} \left(\langle W_j | H(\mathbf{r}) | W_j \rangle + \mu^{-1} ||W_j||_1 \right) \quad \text{s.t.} \quad \langle W_j | W_k \rangle = \delta_{jk}$$

$$||W||_1 = \sum_i |W(\mathbf{r}_i)|$$

- Parameter μ controls the trade-off between compact support and energy accuracy.

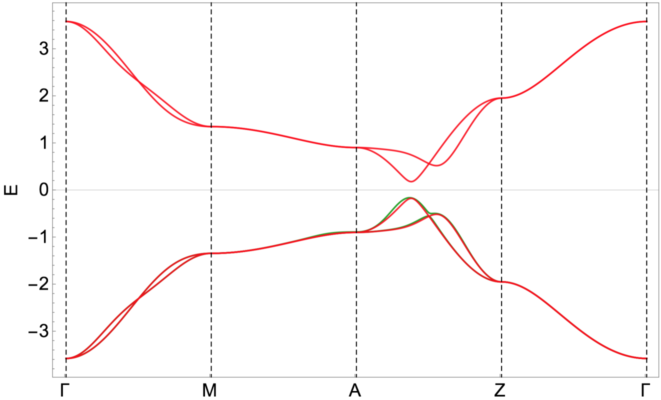
Compressed Wannier Modes for Fu's Model

- Choose intermediate value of μ, a good initial guess, and super-cell of N^3 unit cells.
- Calculate occupied Wannier functions.



- Functions have compact support but structure is not clear.

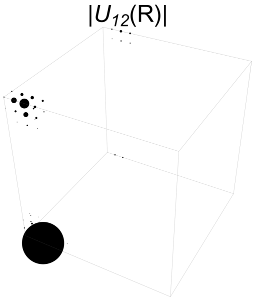
Interpolated Band Structure

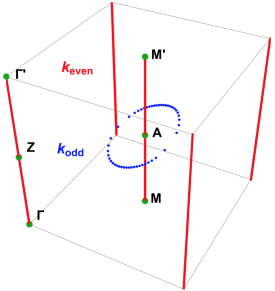


- How can we verify that our Wannier functions have the correct topological properties?

Pfaffian

- Symmetry operator matrix: $U_{ij}(\mathbf{R}) = \langle W_i(\mathbf{r}-\mathbf{R}) | \hat{C}_4 \hat{K} | W_j(\mathbf{r}) \rangle$
- Pfaffian: $\mathrm{Pf}[U_{ij}(\mathbf{k})] = U_{12}(\mathbf{k})$
  - $\rightarrow$ Wannier functions establish smooth gauge in BZ.

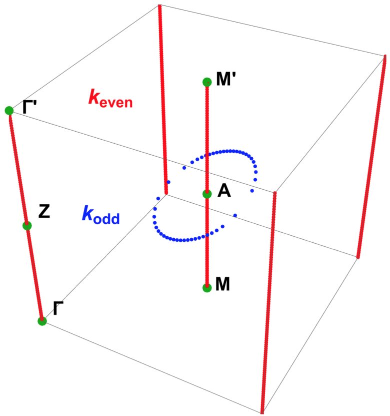




- $\mathbf{k}_{\mathrm{even}} \in \mathbf{k}$, where $U_{12}(\mathbf{k}_{\mathrm{even}}) = 1$
- $\mathbf{k}_{\mathrm{odd}} \in \mathbf{k}$, where $U_{12}(\mathbf{k}_{\mathrm{odd}}) = 0 + 0i$

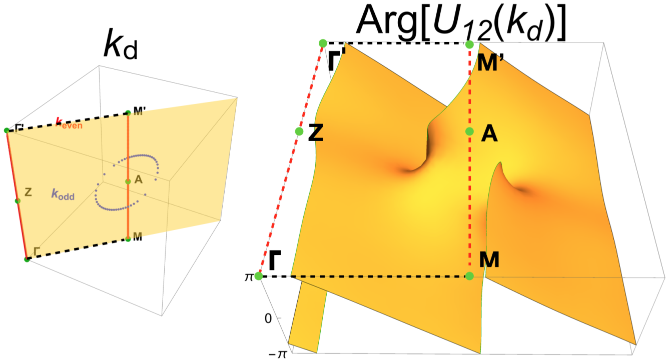
Pfaffian

- Pfaffian: $\mathrm{Pf}[U_{ij}(\mathbf{k})] = U_{12}(\mathbf{k})$



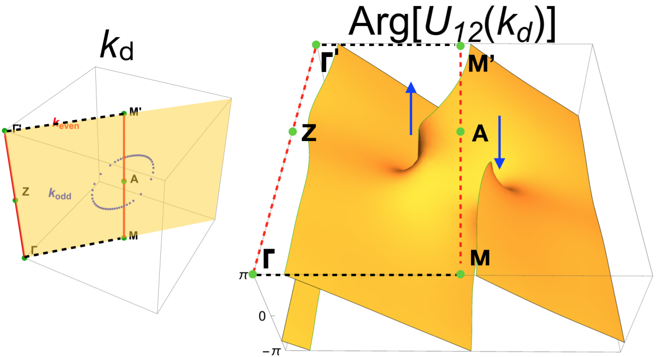
- $\mathbf{k}_{\mathrm{even}}$ is protected by $\hat{C}_4$ symmetry.
- Only gauges that break $\hat{C}_4$ symmetry can remove $\mathbf{k}_{\mathrm{odd}}$.

Pfaffian Phase



- Following our high symmetry countour increases phase by 2π.

Pfaffian Phase

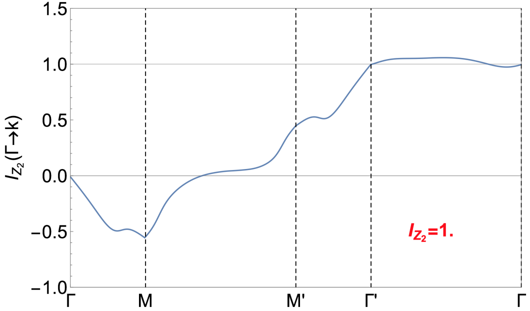


- Complex zeros have opposite winding direction.
- $\mathbf{k}_{\text{even}}$ prevents complex zero annhilation.

Pfaffian Z2 Index

$$I_{Z_2} = \frac{1}{2\pi} \oint_C \nabla_{\mathbf{k}} \mathrm{Im}\Big[\log[U_{21}(\mathbf{k}) + i\delta_{\mathbf{k}}]\Big] d\mathbf{k}$$

- Singularities of the integrand occur when $U_{21}(\mathbf{k})$ is a complex zero.

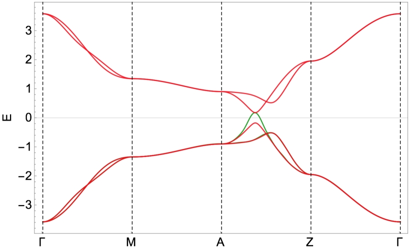


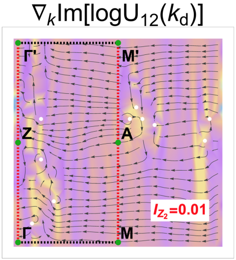
- Practically, we are counting complex zeros within the area of our contour.

Compressed Wannier Modes Inaccuracies

- Calculating compressed Wannier modes requires solving a non-convex minimization problem
- Certain initial guesses can produce significant inaccuracies.

  → Common inaccuracy is undesired conduction character.





Compressed Wannier Modes via Manifold Projection

- We can restrict compressed Wannier modes to only have occupied manifold character.

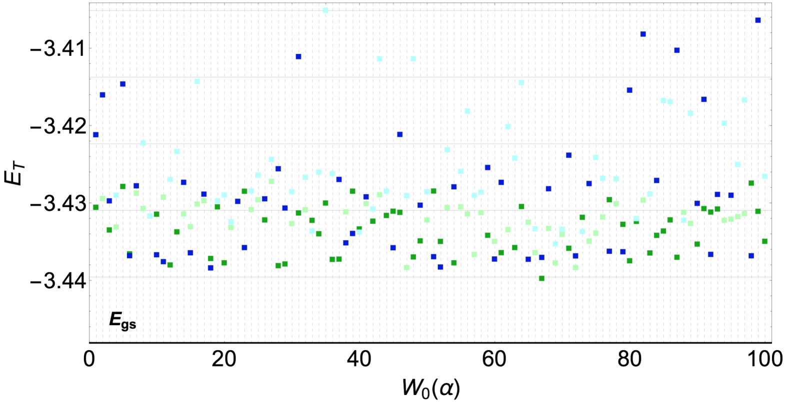
$$E_{\min} = \min_{W} \sum_{j} \left(-\langle W_j | P_V | W_j \rangle + \mu^{-1} || W_j ||_1 \right) \;\; \text{s.t.} \;\; \langle W_j | W_k \rangle = \delta_{jk}$$

$$P_V = \sum_{i \in val} |\phi_i\rangle\langle\phi_i|, \quad H(\mathbf{r})|\phi_i\rangle = E_i|\phi_i\rangle$$

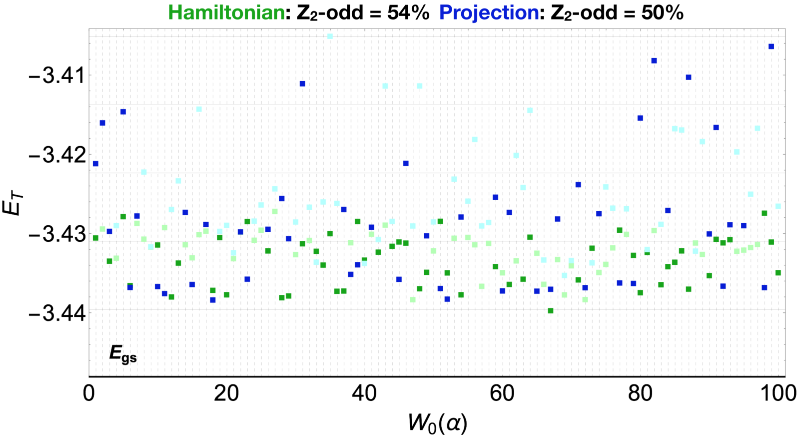
- What are the consequence of changing the energy functional?

Benchmarking Compressed Wannier Mode Methods

- Deal with non-convexity by creating a set of random initial guesses: $W_0(\alpha) = \{\mathbf{r}e^{-(\frac{\mathbf{x}}{\alpha})^2}\}_{i=1}^{n}$
- Calculate Wannier functions for the Hamiltonian and projection methods using $W_0(\alpha)$.
  - $\rightarrow$ $\mu_H \neq \mu_P$; chosen to have comparable E_T-min values.



Benchmarking Compressed Wannier Mode Methods



- Similar topological performance on average.

Conclusions

1. Compressed Wannier modes offer an effective and efficient method for establishing a smooth gauge for topological analysis.

2. Comparing compressed Wannier mode methods
   - → Similar topological performance.
   - → Manifold projection method is faster.
   - → Manifold projection method avoids undesired conduction band character.