Numerical construction of Wannier functions for $\mathbb{Z}_2$ topological insulators

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July 11, 2018

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Introduction

Context:

- Describe electrical properties of crystals (insulator, conductor, semi-conductor).
- Applications in electronics (Silicon transistors, Graphene).
- Wannier functions: localised basis that represents electronic orbitals.

Figure: Graphene, Wannier Function
Introduction

Context:
- Describe electrical properties of crystals (insulator, conductor, semi-conductor).
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Goal
Robust method to construct Wannier functions numerically.

Figure: Graphene, Wannier Function
1 Wannier Functions

2 Numerical constructions of Wannier functions

3 A more robust algorithm
**Bloch decomposition**

**Assumptions:** Born-Oppenheimer, independent electrons. Lattice $\mathcal{R}$, reciprocal lattice $\mathcal{R}'$, Brillouin Zone $\mathcal{B}$.

**Bloch waves:**

\[
\Psi_{n,k}(r) = e^{ik \cdot r} v_{n,k}(r), \quad \text{with } v_{n,k}(r + R) = v_{n,k}(r), \\
\text{and } v_{n,k+\mathbf{K}}(r) = e^{i\mathbf{K} \cdot r} v_{n,k}(r), \quad R \in \mathcal{R}, \quad \mathbf{K} \in \mathcal{R}'
\]

Hamiltonian on Bloch waves: $H_k = \frac{1}{2} \left( -i \nabla + \mathbf{k} \right)^2 + V$.

$H_k$ has compact resolvent: $\varepsilon_{n,k}$ eigenvalues, $v_{n,k}$ eigenvectors, $P_{n,k}$ spectral projectors.

**Time reversal symmetry (bosonic +/ fermionic −)**

\[
P_{-k} = \theta P_k \theta^{-1}, \quad \text{where } \theta \text{ antiunitary such that } \theta^2 = \pm 1.
\]
Topological insulator model in $\mathbb{C}^4$ with Quantum Spin Hall effect, characterized by $\mathbb{Z}_2$ invariant. Satisfies FTRS, includes spin-orbit coupling.

$$H_k = \sum_{a=1}^{5} d_a(k) \Gamma^a + \sum_{a<b=1}^{5} d_{ab}(k) \Gamma^{ab},$$

Gap between the 2 lower bands and the 2 upper ones.

**Figure:** Energy bands for a one-dimensional “zigzag” strip in the (a) QSH phase (b) the insulating phase.
**Assumption:** Isolated set of $N$ bands (gap).

- Introduce the choice of gauge $U(k)$ (unitary):
  \[ u_{n,k} = \sum_{m=1}^{N} U_{mn}^{(k)} v_{m,k}, \]

  \[ u_k = (u_{1,k} \ldots u_{N,k}) \text{ not eigenstates, but span } \text{Ran} \{ v_{n,k} \}. \]

- Wannier functions:
  \[ w_n(r) = \int_{\mathcal{B}} e^{i\mathbf{k} \cdot \mathbf{r}} u_{n,k}(r) d\mathbf{k}. \]

  \[ \{ w_n \}_n \text{ and translations are a basis of } \text{Ran}(\{ u_k \}_k). \]

- Localisation of $w_n$ $\Leftrightarrow$ smoothness of $k \mapsto u_k$. ($\approx$ Fourier).

*Can we choose $U(k)$ such that $k \mapsto u_k$ is smooth and quasi-periodic?*
Problem statement

Problem

Given the Bloch waves $v_k$ (DFT calculations), can we construct a gauge $U(k)$ such that the resulting frame $u_k = v_k U(k)$ is smooth and quasi-periodic ($u_{k+K} = u_k e^{iK \cdot r}$)?

- (P1): Does such a gauge exist?
- (P2): How can we construct it algorithmically?

To simplify notation, $u_{k+K}(r) = u_k(r)$, but results can be adapted in quasi-periodic case.

(P1): Competition between continuity and periodicity, obstruction to existence is of topological nature.
A touch of complex vector bundle topology

**Bloch bundle**

Base space $\mathcal{B}$, fibre $\text{Ran}(P_k)$ is a hermitian vector space.

- In 1D: no topological obstruction.
- In dimension 2 and higher, the ability to construct a continuous frame on the Brillouin zone is determined by topological invariants.

**Chern number**

For dimension $d = 2$, Chern number $c$ contains the topological information.

If $c = 0$, there exists a smooth gauge choice ([Panati’07]).

Bosonic and fermionic time reversal symmetry imply $c = 0$, but continuous FTRS Bloch frame does not necessarily exist.
We consider an insulator, and assume from here on that $c = 0$, so that an appropriate gauge exists.

- Original proof is non-constructive ([Panati’07]).
- Constructive proofs in [Fiorenza-Monaco-Panati’16] and [Cornean-Herbst-Nenciu’16] are not readily implementable (use perturbative arguments).
- Numerical approach: [Marzari-Vanderbilt’97] Minimises iteratively the spread of the Wannier functions, but needs a good initial guess to converge properly.

Can we have our cake and eat it too?
1. Wannier Functions

2. Numerical constructions of Wannier functions

3. A more robust algorithm
First proposed in [Marzari-Vanderbilt’97].

- Spread of the Wannier functions
  \[ \Omega(\{w_n\}) = \sum_{n=1}^{N} \langle w_n| r^2 |w_n\rangle - \langle w_n| r |w_n\rangle^2. \]

- Can be alternatively written in terms of \( u_k \): measures regularity in \( k \) of Bloch waves.

- Gradient descent on spread: maximally-localized Wannier functions, smooth \( u_k \) [Panati-Pisante’11].

- ... Provided good initial guess.

- In original paper, initial guess obtained by projection method.
**Projection method:**

- Reference orbitals given by physical intuition.
- Project reference on the Bloch wave space.
- Normalise the projected frame.

**Figure:** Upper row: random initial guess for a random potential, Bloch frame, and Wannier function (log scale). Lower: result after MV.

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Wannier functions
Parallel transport

Assume $P(t)$ a continuous family of projectors.

### How to build a continuous frame of $\text{Ran}(P(t))$?

- Choose $U(0)$ a basis of $\text{Ran}(P(0))$.
- Propagate according to
  $$U(t + \varepsilon) = P(t + \varepsilon)U(t).$$

In the limit $\varepsilon \to 0$, parallel transport equation

$$\begin{cases}
P(t)\dot{U}(t) = 0, & \forall t \in [0, 1], \\
U^*(t)U(t) = I.
\end{cases}$$
Parallel transport

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**Unitary discretisation**

$$\begin{cases}
\tilde{U}_{n+1} = P(t_{n+1})U_n, \\
U_{n+1} = \tilde{U}_{n+1} \left(\tilde{U}_{n+1}^*\tilde{U}_{n+1}\right)^{-\frac{1}{2}}.
\end{cases}$$
Algorithm in 1D

- Choose $u_0 = v_0$.
- Project $u_0$ on $\text{Ran}(v_{\delta k})$ and renormalise to obtain $u_{\delta k}$.
- Iterate the projections until $u_1$ (parallel transport).
- $u_0$ can be different from $u_1$, but they span the same space. Hence, we can find a unitary matrix $\text{Obs}$, such that $u_1 = u_0 \text{Obs}$.
- We can then unwind the frame by $
abla^* u_k = u_k \text{Obs}^{-k}$.

Then $k \mapsto \nabla^* u_k$ is continuous and periodic.

1D case: known since the 60’s (Kohn, des Cloizeaux).
Algorithm in 2D

- Apply the 1D algorithm to $\mathbf{v}_{0,k_2}$, and put the result in $\mathbf{u}_{0,k_2}$.
- Propagate $\mathbf{u}_{k_1,k_2}$ until $k_1 = 1$. Then $\mathbf{u}_{k_1,k_2}$ is $k_2$-periodic, but not $k_1$-periodic.
- Define an obstruction matrix such that $\mathbf{u}_{1,k_2} = \mathbf{u}_{0,k_2} \text{Obs}(k_2)$.
- Build a continuous homotopy $\text{Obs}(k_1, k_2)$ s.t.
  \[
  \text{Obs}(0, k_2) = \mathbf{I}, \quad \text{Obs}(1, k_2) = \text{Obs}(k_2).
  \]
- Unwind the frame by
  \[
  \hat{\mathbf{u}}_{k_1,k_2} = \text{Obs}(k_1, k_2)^* \mathbf{u}_{k_1,k_2}.
  \]
Unitary path homotopy

Fact
If Chern = 0, one can choose \( \text{Obs}(k_2) \in SU(N) \).

\( SU(N) \) : simply-connected, so all paths are contractible.

How to construct a continuous homotopy in \( SU(N) \)?

\[
\text{Obs}(k_1, k_2) = \exp \left( k_1 \log \text{Obs}(k_2) \right),
\]

Simple counter example (Kane-Mele has similar behavior):

\[
\text{Obs}(k_2) = \begin{pmatrix}
\exp(2i\pi k_2) & 0 \\
0 & \exp(-2i\pi k_2)
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Logarithm preserves the diagonal structure, and diagonal \( SU(N) \) is not simply connected.
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Need to break the symmetry!
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Parallel transport algorithm

**General idea**

Break the $SU(N)$ homotopy into $N$ consecutive homotopies on spheres.

- Contract the first column continuously to a point.
- Parallel transport the other columns in the orthogonal subspace.
- Contract the second column...
- The last column has only a phase degree of freedom, which can be unwind because $c = 0$.

This process yields a continuous homotopy, and breaks any additional symmetries.
Consider the path of the first column $T^1 \ni s \rightarrow u_1(s) \in S^N_C$, where

$$S^N_C = \left\{ z \in \mathbb{C}^N \mid \sum |z_i|^2 = 1 \right\}.$$  

**Fact**

For $N > 1$, $S^N_C$ is simply connected.

To construct a homotopy,

- Find a point on the sphere $u_1$ such that $u_1(s) + \overline{u_1} \neq 0$.
- Interpolate $u_1(s)$ as follows

$$u_1(t, s) = \frac{tu_1(s) + (1 - t)\overline{u_1}}{\|tu_1(s) + (1 - t)\overline{u_1}\|}.$$  

Parallel transport $(u_2(s), \ldots u_N(s)) \perp u(t, s)$

Gives $u_2(t, s)$, where $u_2(1, s) \perp u_1$. 

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Gives $u_2(t, s)$, where $u_2(1, s) \perp \underline{u_1}$.

$\Rightarrow$ Contract $u_2(1, s) \in S^{N-1}_C$. ...
Results for Kane-Mele model

Figure: $[\text{Re}(\text{Obs}_{11}), \text{Im}(\text{Obs}_{11})]$: Unwinding the obstruction
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**Results**

**Figure:** Local Ω, regularity of Bloch frame obtained by log homotopy

**Figure:** Local Ω, regularity of Bloch frame obtained by parallel transport homotopy

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Wannier functions
What we did

- Systematic approach to build a continuous gauge choice, proven to work.
Conclusion

What we did

- Systematic approach to build a continuous gauge choice, proven to work.
- The continuous gauge can be refined to a smooth frame (using the Marzari-Vanderbilt algorithm, for example).

Thank you for your attention!

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- Systematic approach to build a continuous gauge choice, proven to work.
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- More general than the Kane-Mele case.

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