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

Sami Siraj-dine

July 11, 2018

CERMICS, École des Ponts
Advisors: Éric Cancès, Clotilde Fermanian, Antoine Levitt.

Context:

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

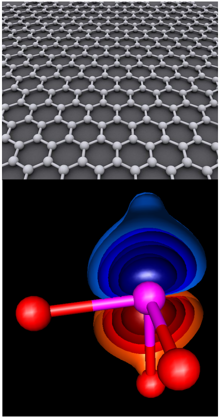


Figure: Graphene, Wannier Function

Introduction

Context:

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

Goal

Robust method to construct Wannier functions numerically.

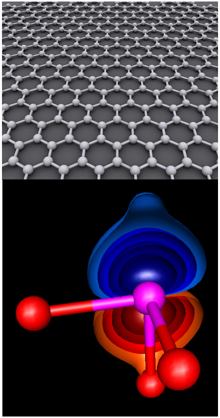


Figure: Graphene, Wannier Function

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

Bloch waves:

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

Hamiltonian on Bloch waves: $H_{\mathbf{k}} = \frac{1}{2}\left(-i\nabla + \mathbf{k}\right)^2 + V$.
$H_{\mathbf{k}}$ has compact resolvent: $\varepsilon_{n,\mathbf{k}}$ eigenvalues, $v_{n,\mathbf{k}}$ eigenvectors, $P_{n,\mathbf{k}}$ spectral projectors.

Time reversal symmetry (bosonic $+$/ fermionic $-$)

$$P_{-k} = \theta P_k \theta^{-1}, \quad \text{where } \theta \text{ antiunitary such that } \theta^2 = \pm 1.$$

[Kane-Mele'05]

Topological insulator model in $\mathbb{C}^4$ with Quantum Spin Hall effect, characterized by $\mathbb{Z}_2$ invariant. Satisfies FTRS, includes spin-orbit coupling.

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

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

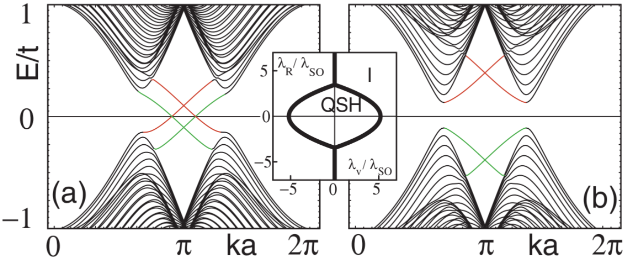


Figure: Energy bands for a one-dimensional "zigzag" strip in the (a) QSH phase (b) the insulating phase.

Assumption: Isolated set of N bands (gap).

- Introduce the choice of gauge $\mathbf{U}(\mathbf{k})$ (unitary):

$$u_{n,\mathbf{k}} = \sum_{m=1}^{N} U_{mn}^{(\mathbf{k})} v_{m,\mathbf{k}},$$

$\mathbf{u}_{\mathbf{k}} = (u_{1,\mathbf{k}} \dots u_{N,\mathbf{k}})$ not eigenstates, but span $\mathrm{Ran}\,\{v_{n,\mathbf{k}}\}$.

- Wannier functions:

$$w_n(\mathbf{r}) = \int_{\mathcal{B}} \mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}} u_{n,\mathbf{k}}(\mathbf{r}) \mathrm{d}\mathbf{k}.$$

$\{w_n\}_n$ and translations are a basis of $\mathrm{Ran}(\{\mathbf{u}_k\}_{\mathbf{k}})$.

- Localisation of $w_n \Leftrightarrow$ smoothness of $\mathbf{k} \mapsto \mathbf{u}_{\mathbf{k}}$. ($\simeq$ Fourier).

Can we choose $\mathbf{U}(\mathbf{k})$ *such that* $\mathbf{k} \mapsto \mathbf{u}_{\mathbf{k}}$ *is smooth and quasi-periodic?*

Problem statement

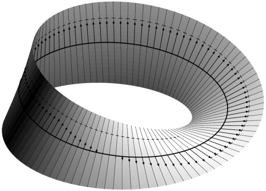
Problem

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

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

To simplify notation, $\mathbf{u_{k+K}}(\mathbf{r}) = \mathbf{u_k}(\mathbf{r})$, 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 $\mathrm{Ran}(P_k)$ 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.

(P2): How to construct a gauge?

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?

Marzari-Vanderbilt algorithm

First proposed in [Marzari-Vanderbilt'97].

- Spread of the Wannier functions
$$\Omega(\{w_n\}) = \sum_{n=1}^{N} \langle w_n | \mathbf{r}^2 | w_n \rangle - \langle w_n | \mathbf{r} | w_n \rangle^2 .$$
- Can be alternatively written in terms of $\mathbf{u_k}$: measures regularity in $\mathbf{k}$ of Bloch waves.
- Gradient descent on spread: maximally-localized Wannier functions, smooth $\mathbf{u_k}$ [Panati-Pisante'11].
- ... Provided good initial guess.
- In original paper, initial guess obtained by projection method.

MV algorithm: Initial guess

Projection method:

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

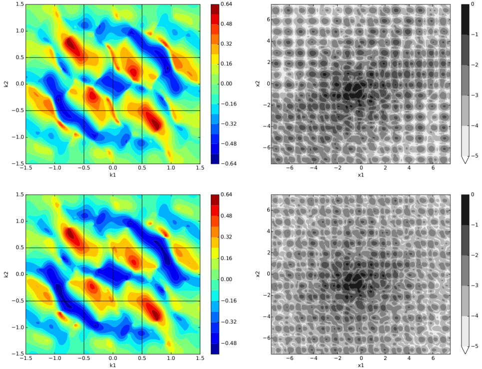


Figure: Upper row: random initial guess for a random potential, Bloch frame, and Wannier function (log scale). Lower: result after MV.

Parallel transport

Assume $\mathbf{P}(t)$ a continuous family of projectors.

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

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

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

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

Parallel transport

Assume $\mathbf{P}(t)$ a continuous family of projectors.

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

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

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

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

Unitary discretisation

$$\begin{cases} \widetilde{\mathbf{U}}_{n+1} = \mathbf{P}(t_{n+1})\mathbf{U}_n, \\ \mathbf{U}_{n+1} = \widetilde{\mathbf{U}}_{n+1}\left(\widetilde{\mathbf{U}}_{n+1}^*\widetilde{\mathbf{U}}_{n+1}\right)^{-\frac{1}{2}}. \end{cases}$$

Algorithm in 1D

- Choose $\mathbf{u}_0 = \mathbf{v}_0$.
- Project $\mathbf{u}_0$ on $\mathrm{Ran}(\mathbf{v}_{\delta k})$ and renormalise to obtain $\mathbf{u}_{\delta k}$.
- Iterate the projections until $\mathbf{u}_1$ (parallel transport).
- $\mathbf{u}_0$ can be different from $\mathbf{u}_1$, but they span the same space. Hence, we can find a unitary matrix **Obs**, such that $\mathbf{u}_1 = \mathbf{u}_0 \mathbf{Obs}$.
- We can then unwind the frame by
$$\widehat{\mathbf{u}}_k = \mathbf{u}_k \mathbf{Obs}^{-k}.$$
Then $\mathbf{k} \mapsto \widehat{\mathbf{u}}_\mathbf{k}$ 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 $\mathbf{u}_{1,k_2} = \mathbf{u}_{0,k_2}\mathbf{Obs}(k_2)$.
- Build a continuous homotopy $\mathbf{Obs}(k_1, k_2)$ s.t.
$$\mathbf{Obs}(0, k_2) = \mathbf{I}, \quad \mathbf{Obs}(1, k_2) = \mathbf{Obs}(k_2).$$
- Unwind the frame by
$$\widehat{\mathbf{u}}_{k_1,k_2} = \mathbf{Obs}(k_1, k_2)^* \mathbf{u}_{k_1,k_2}.$$

Unitary path homotopy

Fact

If Chern $= 0$, one can choose $\mathbf{Obs}(k_2) \in \mathcal{SU}(N)$.

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

How to construct a continuous homotopy in $\mathcal{SU}(N)$?

$$\mathbf{Obs}(k_1, k_2) = \exp\left(k_1 \log \mathbf{Obs}(k_2)\right),$$

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

$$\mathbf{Obs}(k_2) = \begin{pmatrix} \exp(2i\pi k_2) & 0 \\ 0 & \exp(-2i\pi k_2) \end{pmatrix}$$

Logarithm preserves the diagonal structure, and diagonal $\mathcal{SU}(N)$ is not simply connected.

Unitary path homotopy

Fact

If Chern $= 0$, one can choose $\mathbf{Obs}(k_2) \in \mathcal{SU}(N)$.

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

How to construct a continuous homotopy in $\mathcal{SU}(N)$?

$$\mathbf{Obs}(k_1, k_2) = \exp\left(k_1 \log \mathbf{Obs}(k_2)\right),$$

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

$$\mathbf{Obs}(k_2) = \begin{pmatrix} \exp(2i\pi k_2) & 0 \\ 0 & \exp(-2i\pi k_2) \end{pmatrix}$$

Logarithm preserves the diagonal structure, and diagonal $\mathcal{SU}(N)$ is not simply connected.

Need to break the symmetry!

Parallel transport algorithm

General idea

Break the $\mathcal{SU}(N)$ 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.

Contraction of the columns on the sphere

Consider the path of the first column $\mathbb{T}^1 \ni s \to \mathbf{u}_1(s) \in \mathbb{S}^N_{\mathbb{C}}$, where

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

Fact

For $N > 1$, $\mathbb{S}^N_{\mathbb{C}}$ is simply connected.

To construct a homotopy,

- Find a point on the sphere $\underline{\mathbf{u}_1}$ such that $\mathbf{u}_1(s) + \underline{\mathbf{u}_1} \neq 0$.
- Interpolate $\mathbf{u}_1(s)$ as follows

$$\mathbf{u}_1(t,s) = \frac{t\mathbf{u}_1(s) + (1-t)\underline{\mathbf{u}_1}}{\|t\mathbf{u}_1(s) + (1-t)\underline{\mathbf{u}_1}\|}.$$

Parallel transport $(\mathbf{u}_2(s), \ldots \mathbf{u}_N(s)) \perp \mathbf{u}(t,s)$

Gives $\mathbf{u}_2(t,s)$, where $\mathbf{u}_2(1,s) \perp \underline{\mathbf{u}_1}$.

Contraction of the columns on the sphere

Consider the path of the first column $\mathbb{T}^1 \ni s \to \mathbf{u}_1(s) \in \mathbb{S}^N_{\mathbb{C}}$, where

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

Fact

For $N > 1$, $\mathbb{S}^N_{\mathbb{C}}$ is simply connected.

To construct a homotopy,

- Find a point on the sphere $\underline{\mathbf{u}_1}$ such that $\mathbf{u}_1(s) + \underline{\mathbf{u}_1} \neq 0$.
- Interpolate $\mathbf{u}_1(s)$ as follows

$$\mathbf{u}_1(t,s) = \frac{t\mathbf{u}_1(s) + (1-t)\underline{\mathbf{u}_1}}{\|t\mathbf{u}_1(s) + (1-t)\underline{\mathbf{u}_1}\|}.$$

Parallel transport $(\mathbf{u}_2(s), \ldots \mathbf{u}_N(s)) \perp \mathbf{u}(t,s)$

Gives $\mathbf{u}_2(t,s)$, where $\mathbf{u}_2(1,s) \perp \underline{\mathbf{u}_1}$.
$\Rightarrow$ Contract $\mathbf{u}_2(1,s) \in \mathbb{S}^{N-1}_{\mathbb{C}}$...

Results for Kane-Mele model

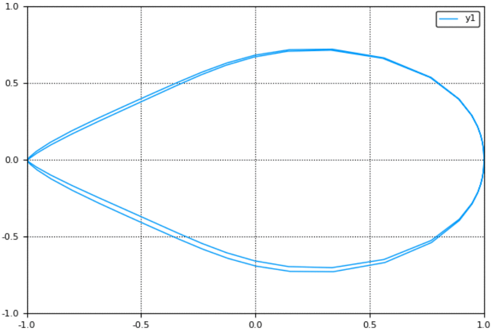


Figure: $[\mathrm{Re}(Obs_{11}), \mathrm{Im}(Obs_{11})]$: Unwinding the obstruction

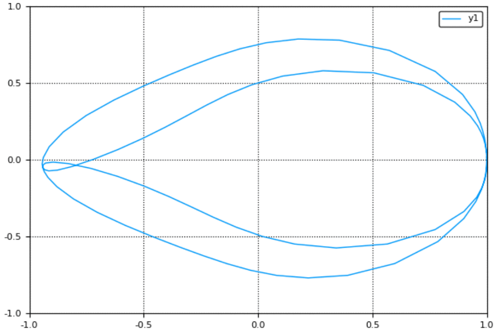


Figure: $[\mathrm{Re}(Obs_{11}), \mathrm{Im}(Obs_{11})]$: Unwinding the obstruction

Results for Kane-Mele model

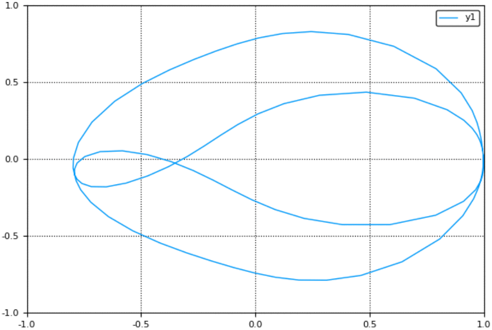


Figure: $[\mathrm{Re}(Obs_{11}), \mathrm{Im}(Obs_{11})]$: Unwinding the obstruction

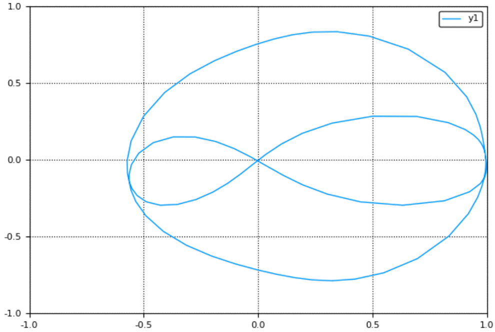


Figure: $[\mathrm{Re}(Obs_{11}), \mathrm{Im}(Obs_{11})]$: Unwinding the obstruction

Results for Kane-Mele model

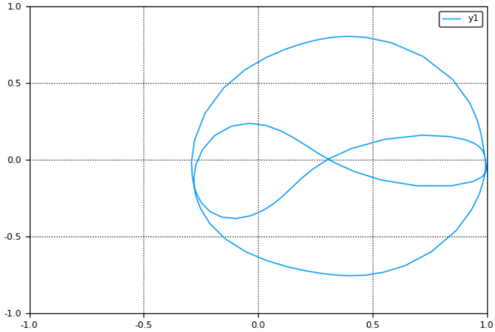


Figure: $[\mathrm{Re}(\mathit{Obs}_{11}), \mathrm{Im}(\mathit{Obs}_{11})]$: Unwinding the obstruction

Results for Kane-Mele model

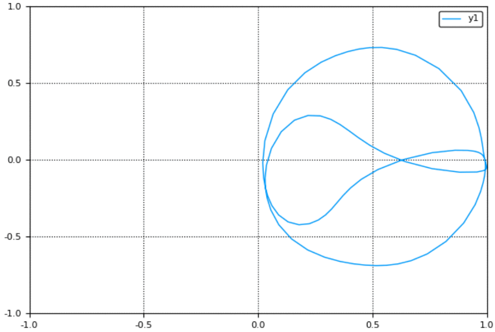


Figure: $[\mathrm{Re}(Obs_{11}), \mathrm{Im}(Obs_{11})]$: Unwinding the obstruction

Results for Kane-Mele model

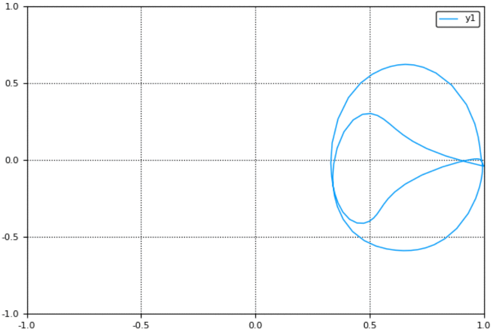


Figure: $[\mathrm{Re}(Obs_{11}), \mathrm{Im}(Obs_{11})]$: Unwinding the obstruction

Results for Kane-Mele model

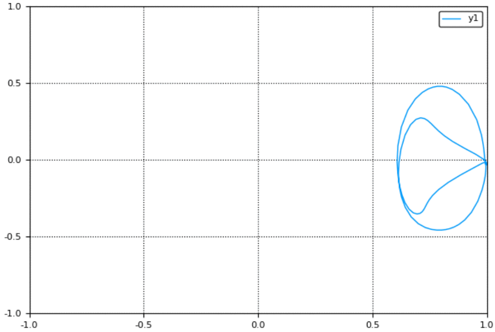


Figure: $[\mathrm{Re}(Obs_{11}), \mathrm{Im}(Obs_{11})]$: Unwinding the obstruction

Results for Kane-Mele model

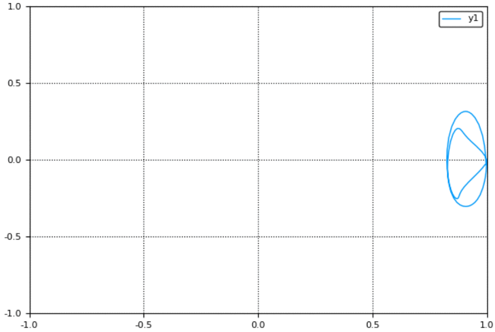


Figure: $[\mathrm{Re}(Obs_{11}), \mathrm{Im}(Obs_{11})]$: Unwinding the obstruction

Results for Kane-Mele model

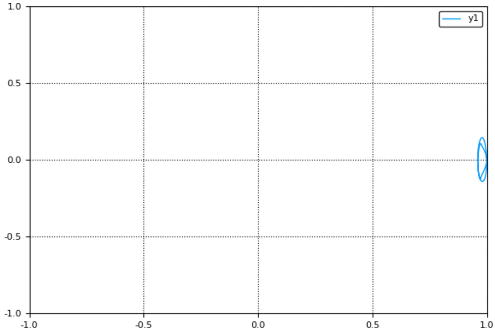


Figure: $[\mathrm{Re}(Obs_{11}), \mathrm{Im}(Obs_{11})]$: Unwinding the obstruction

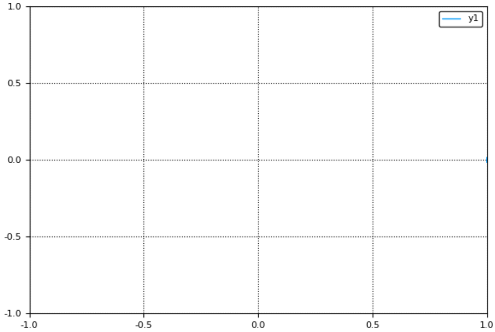


Figure: $[\mathrm{Re}(Obs_{11}), \mathrm{Im}(Obs_{11})]$: Unwinding the obstruction

Results

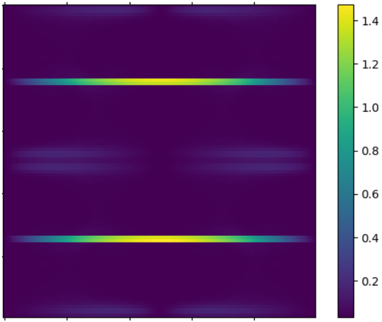


Figure: Local Ω, regularity of Bloch frame obtained by log homotopy

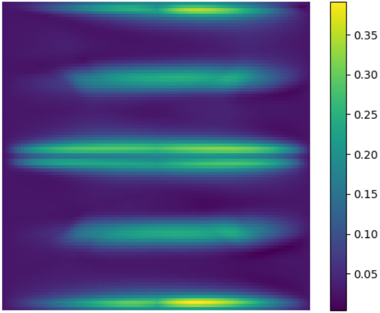


Figure: Local Ω, regularity of Bloch frame obtained by parallel transport homotopy

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).

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).
- More general than the Kane-Mele case.

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).
- More general than the Kane-Mele case.
- Only holds for insulators with $c = 0$ (regular or topological).

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).
- More general than the Kane-Mele case.
- Only holds for insulators with $c = 0$ (regular or topological).

Thank you for your attention!