Wannier functions for insulators and metals

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Copenhagen

Interpolation of eigenvalues

Given $H(k)$ Hermitian matrix, very large, smooth and periodic in a 3D box, how can we efficiently interpolate some of its eigenvalues $\lambda_n(k)$?

Application of interest: periodic quantum system.
$H(k) = (-i\nabla + k)^2 + V$ with periodic boundary conditions on the unit cell. Box = Brillouin zone
(H(k) is not periodic, but almost; pretend it is for simplicity)

For a smooth function $f(k)$:

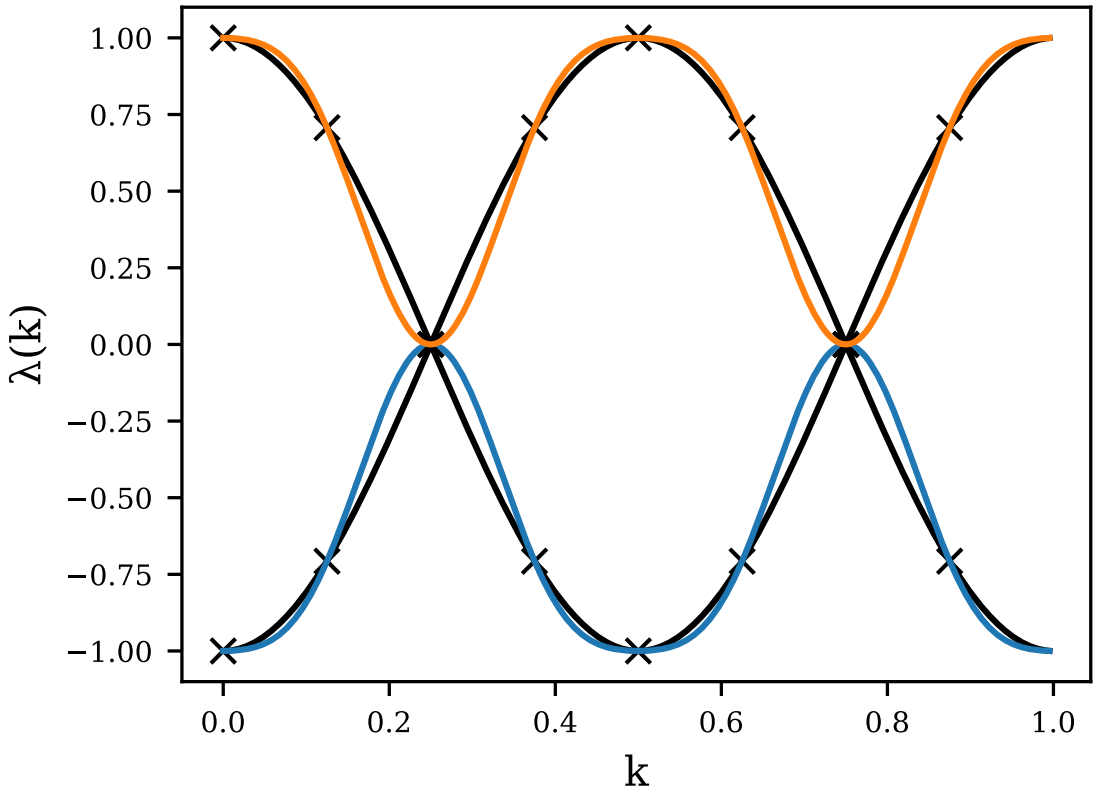
Fourier interpolation

Compute f at N^d equispaced points, expand f in Fourier series and fit its first Fourier coefficients.

Efficient (FFTs) and accurate (smoothness $\Leftrightarrow$ decay of Fourier coefficients $\Leftrightarrow$ interpolation accuracy)

$\Rightarrow$ Fourier interpolation on $\lambda_n(k)$ for all n of interest?

Eigenvalue crossings



$$H(k) = \begin{pmatrix} \cos(2\pi k) & 0 \\ 0 & -\cos(2\pi k) \end{pmatrix}$$

Eigenvalue crossings destroy regularity and produce Gibbs-like oscillations. "Connecting bands" is impossible in $d \geq 2$

$\Rightarrow$ Interpolate H directly. But H is too big...

Wannier functions without Wannier functions

Suppose we are interested in the first N eigenvalues λ_n of $H(k)$, $N \ll \dim H(k)$. If we can find $v_n(k)$ orthogonal basis of the spectral subspace associated with $\lambda_n(k)$, then

$$\widetilde{H}_{mn}(k) = \langle v_m(k), H(k) v_n(k) \rangle$$

has eigenvalues $\lambda_1(k), \ldots, \lambda_N(k)$.
$\Rightarrow$ Form the NxN matrix $\widetilde{H}$, interpolate its elements, and diagonalize the interpolated matrices

- The v_n are **not** eigenvectors
- The v_n are highly non-unique: gauge choice $v'_n(k) = \sum_{m=1}^{N} v_m(k) U_{mn}(k)$ with a unitary $U(k)$
- The interpolation will be accurate if $v_n(k)$ is smooth and periodic
- This implies that the eigenvalues $\lambda_1, \ldots, \lambda_N$ are isolated from $\lambda_{N+1}, \ldots$ for all k (e.g. occupied bands of an insulator)
- By Bloch transform, $v_n \Leftrightarrow$ Wannier functions, $\widetilde{H}_{mn} \Leftrightarrow$ tight-binding model, smoothness $\Leftrightarrow$ locality

Smooth continuous eigenvectors and topology

Case $N = 1$: given a smooth and periodic $H(k)$ whose first eigenvalue is separated from the others, can one find a normalized, smooth and periodic eigenvector $v_1(k)$?

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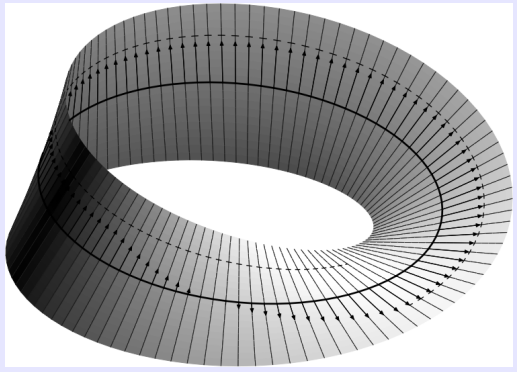
Not always! For instance, if we require $v_1(k)$ to be real:

Simplest example of a topological obstruction: real eigenvectors

$$H(k) = \begin{pmatrix} -\cos(2\pi k) & \sin(2\pi k) \\ \sin(2\pi k) & \cos(2\pi k) \end{pmatrix}$$

$$\lambda_1(k) = -1, v_1(k) = (\cos(\pi k), \sin(\pi k))$$

$v_1(0) = -v_1(1)$!



Allowing complex eigenvectors, one can choose $v(k) = e^{i\pi k}(\cos(\pi k), \sin(\pi k))$ to cancel the flip with a phase.
OK in 1D, not in $d \geq 2$: Chern numbers.

Topological obstructions

Theorem

Let P be a smooth finite-rank projector on a two-dimensional compact connected surface S. Then the following are equivalent

- *There exists a smooth orthogonal basis v_n spanning* Ran P
- *The Chern number*

$$\boxed{Ch(P,S) := \frac{1}{2\pi}\int_S \mathcal{F} \in \mathbb{Z}}$$

vanishes, where $\mathcal{F} := -i\,\mathrm{Tr}(P\,dP \wedge dP)$ is the Berry curvature 2-form

- Application to periodic Schrödinger operators: $S = T^2$ 2-torus
- For $-\Delta + V$ systems (no magnetic field): $\mathcal{F}(-k) = -\mathcal{F}(k)$
- Localized Wannier functions $\Leftrightarrow$ smooth and periodic v_n $\Leftrightarrow$ zero Chern number $\Leftrightarrow$ no quantum Hall effect [TKNN '82, Panati '07, ...]
- Two insulators with different Chern numbers cannot be connected smoothly: **topological phases of matter** (Nobel 2016)

$\Rightarrow$, with $S = T^2$

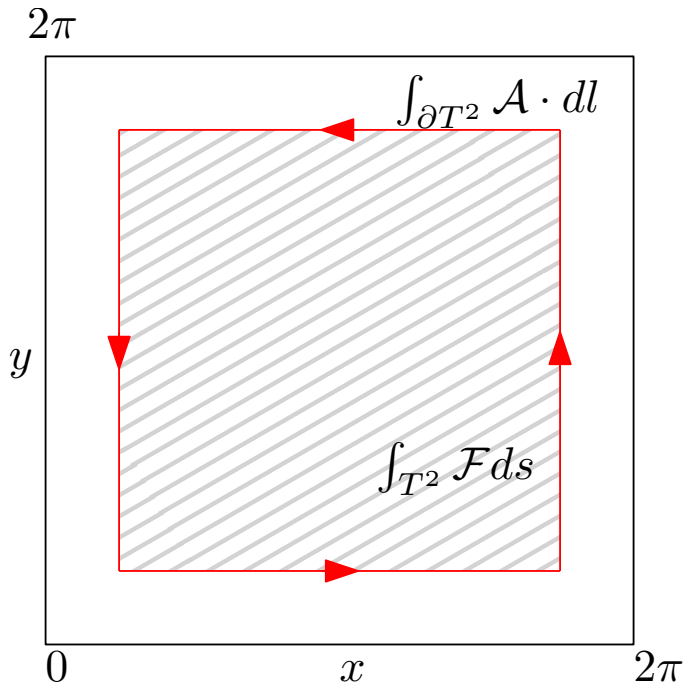
If $v_1, \ldots, v_N$ is smooth and periodic, let $\mathcal{A}_{mn} := -i \langle v_m, \nabla v_n \rangle$ be its Berry connection, then

$$\mathcal{F} := -i \operatorname{Tr}(P[\partial_x P, \partial_y P]) = \operatorname{curl} \operatorname{Tr} \mathcal{A}$$

$\mathcal{A}$ is gauge-dependent (depends on v), $\mathcal{F}$ is **not** (depends only on P)

By Stokes

$$2\pi Ch(P, S) = \int_{T^2} \mathcal{F} ds = \int_{\partial T^2} \mathcal{A} \cdot dl = 0 \quad \square$$



$\Leftarrow$, with $S = T^1$

Begin with the 1D case, $S = T^1 \simeq [0,1]$

- Pick $v_1, \ldots, v_N$ at 0
- Propagate to $[0,1]$ by parallel transport

$$\boxed{\frac{dv}{dx} = (1-P)\frac{dP}{dx}v}$$

- $v(1) \neq v(0)$, but both span the same space $\operatorname{Ran} P(0) = \operatorname{Ran} P(1)$: there is $U \in \mathrm{U}(N)$ such that

$$v_i(1) = \sum_{j=1}^{N} v_j(0) U_{ji}$$

$$v(1) = v(0)U$$

- Set

$$\widetilde{v}(x) = v(x)e^{-x \log U}$$

and we have

$$\widetilde{v}(1) = v(1)U^* = v(0) = \widetilde{v}(0)$$

$\Leftarrow$, with $S = T^2$

Now with $S = T^2$

- We know how to solve the problem in 1D (see before), so assume v is continuous and periodic on $y = 0$
- Use parallel transport in y: $\frac{dv}{dy} = (1 - P)\frac{dP}{dy}v$
- v is continuous on $[0, 1] \times (0, 1)$, but $v(x, 1) \neq v(x, 0)$

$$\boxed{v(x, 1) = v(x, 0)U(x)}$$

- $U(1) = U(0)$, but trouble if $U(x)$ winds, e.g. $U(x) = e^{2\pi i x}$
- We compute

$$\mathcal{A}_x(x, 1) = -iU(x)^* U'(x) + U(x)^* \mathcal{A}_x(x, 0)U(x)$$

and by Stokes

$$\begin{aligned} W(\det U) &= \frac{1}{2\pi i}\int_0^1 \mathrm{Tr}(U(x)^* U'(x))dx \\ &= \frac{1}{2\pi}\int_{\partial T^2} \mathcal{A} \cdot dl = \frac{1}{2\pi}\int_{T^2} \mathcal{F} ds = 0 \end{aligned}$$

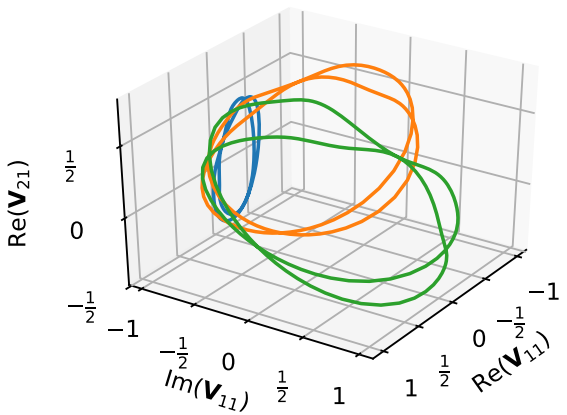
$\Leftarrow$, with $S = T^2$

$$v(x,1) = v(x,0)U(x)$$
$$W(\det U) = 0$$

- If $N = 1$, we are done: $U \in \mathbb{C}$ does not wind and so $U(x) = e^{2\pi i\theta(x)}$ with $\theta(x)$ continuous and periodic:

  $$\widetilde{v}(x,y) = v(x,y)e^{-2\pi iy\theta(x)}$$

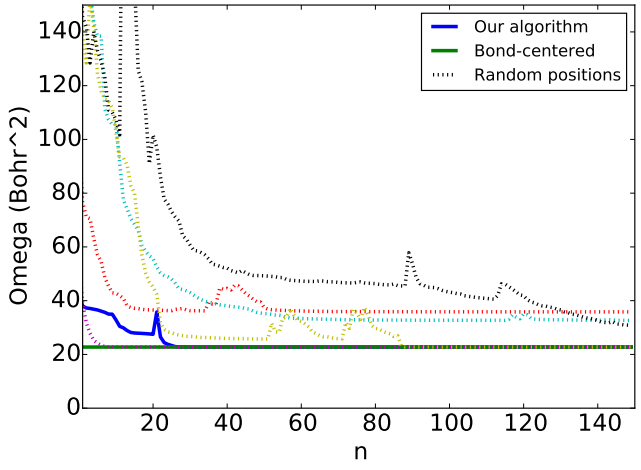
  is continuous and periodic.
- Otherwise, use $U(x) = \det U(x)\frac{U(x)}{\det U(x)}$ and the simple-connectedness of $\mathrm{SU}(N)$



Wannier functions in practice

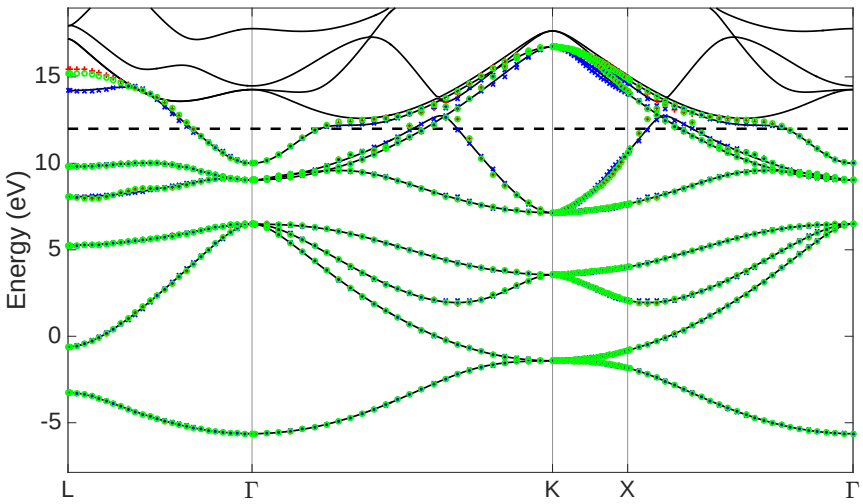
In practice, how to find good v_n on a discrete grid?

- [Marzari/Vanderbilt '97]: maximally-localized Wannier functions
- Define a smoothness functional Ω on the v_n, and optimize iteratively
- Very efficient in practice if a good starting point is known (guessed from chemical properties of the system) $\Rightarrow$ often tricky...
- Recent work on alternative schemes to automatically get a good starting point
  1. pick good columns of the density matrix [Damle/Lin/Ying '15]
  2. mimic the proof of the above theorem [Cancès/Levitt/Stoltz/Panati '17], [Gontier/Levitt/Siraj-Dine '18]



Metals

As we've seen, one can get smooth v_n as long as $\lambda_1, \ldots, \lambda_N$ are isolated from the rest.
And yet... [Souza/Marzari/Vanderbilt '01]



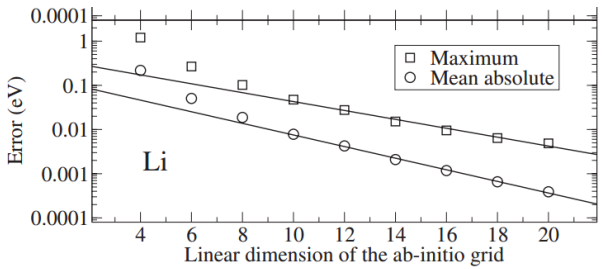


FIG. 6. Convergence of the Wannier-interpolated band energies as a function of the linear dimensions $N_0^{1/3}$ of the *ab initio* **q**-point grid. We plot the maximum error (squares) and mean absolute error

Even the subspace is not smooth! How does this work?

Wannier functions for metals

Using the same definition as before will not yield smooth v_n, we have to generalize

Disentangled Wannier functions

Find $v_1, \ldots, v_{N+N_{\text{extra}}}$ that are smooth and span the spectral subspace $\operatorname{Ran} P_N$ associated with $\lambda_1, \ldots, \lambda_N$

If $\lambda_1, \ldots, \lambda_{N+N_{\text{extra}}}$ are isolated from the rest, then this is the same problem as before.
If not, can this be done? How big must N_{extra} be?

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If not, can this be done? How big must N_{extra} be?

Theorem (Cornean/Gontier/Levitt/Monaco '18)

Let $d = 3$, assume time-reversal symmetry, and let

$$K_n = \{k, \lambda_n(k) = \lambda_{n+1}(k)\}$$

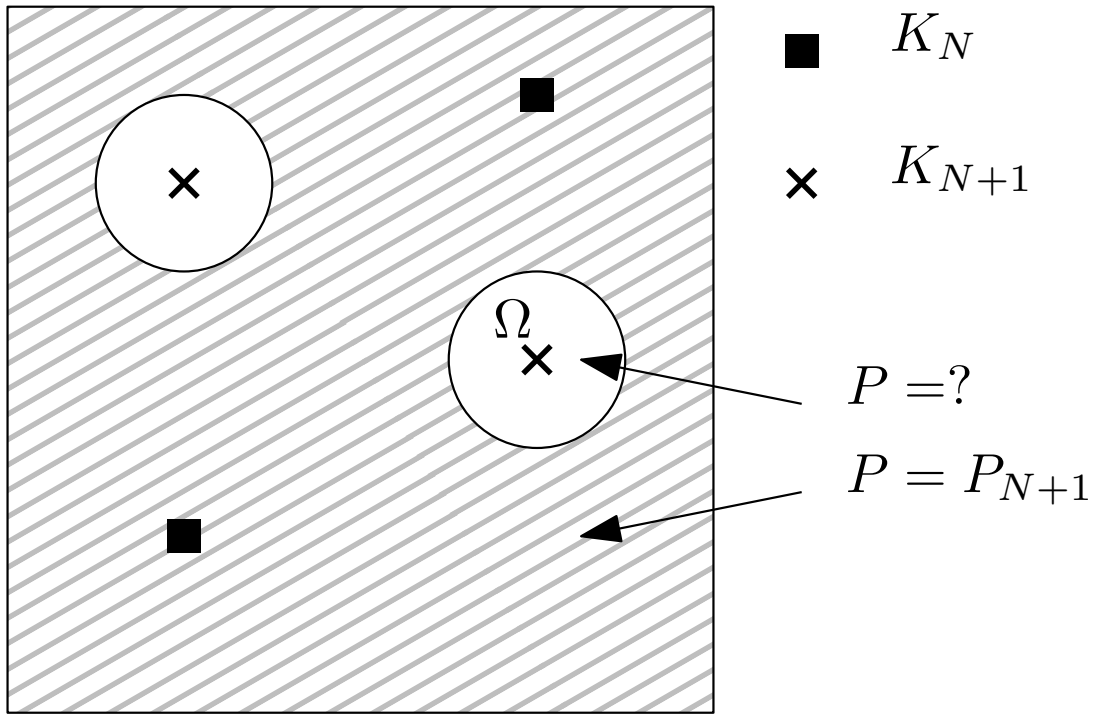
If K_N and K_{N+1} are unions of points and curves, and $K_N \cap K_{N+1} = \emptyset$, then there exist such v_n, with $N_{\text{extra}} = 1$.

Continuation of projectors

- To build the v_n, first build P smooth such that $\operatorname{Ran} P_N \subset \operatorname{Ran} P$, and then find a basis of that. Problem: crossings

$$K_n = \{k, \lambda_n(k) = \lambda_{n+1}(k)\}$$

- P_N is smooth outside of K_N, P_{N+1} is smooth outside of K_{N+1}
- $\Rightarrow$ choose $P = P_{N+1}$ outside of neighborhoods of K_{N+1}, and continue it inside



Continuation of projectors

Problem in 3D

Let Ω be a connected open set in $\mathbb{R}^3$. Then, if P is smooth on Ω, $Ch(P, \partial\Omega) = 0$.

Proof: $\int_{\partial\Omega} \mathcal{F} = \int_{\Omega} d\mathcal{F} = 0$. □

Nonzero Chern numbers are typical at generic crossings (*Weyl points*)

$$H(k) = k \cdot \sigma = \begin{pmatrix} k_3 & k_1 - ik_2 \\ k_1 + ik_2 & -k_3 \end{pmatrix}, \quad \lambda_{\pm}(k) = \pm|k|$$

The projector P_- on the first eigenvector on $\partial\Omega = \{|k| = 1\}$ has Chern number (Weyl charge) $Ch(P_-, \partial\Omega) = -1$: it cannot be continued inside!

In fact this is a characterization:

Theorem

Let P be smoothly defined on $\partial\Omega$. The following are equivalent:

- *$Ch(P, \partial\Omega) = 0$ (recall $\Leftrightarrow$ P has a smooth orthogonal basis on $\partial\Omega$)*
- *P has a smooth continuation to Ω*

Sketch of proof

Strategy of proof when Ω is a ball: build a smooth basis on the sphere, and continue it inside
When Rank $P = 1$,

Lemma ($\pi_2(S_{2M-1})$ is trivial)

If $v \in S_{2M-1} = \{u \in \mathbb{C}^M, |u| = 1\}$ is smoothly defined on the sphere, then it can be smoothly continued inside

Proof for $M \geq 2$: $2M - 1 > 2$, so there is $v^* \in S_{2M-1}$ such that $v(\omega) \neq -v^*$ for ω on the sphere. For $k = r\omega$, let

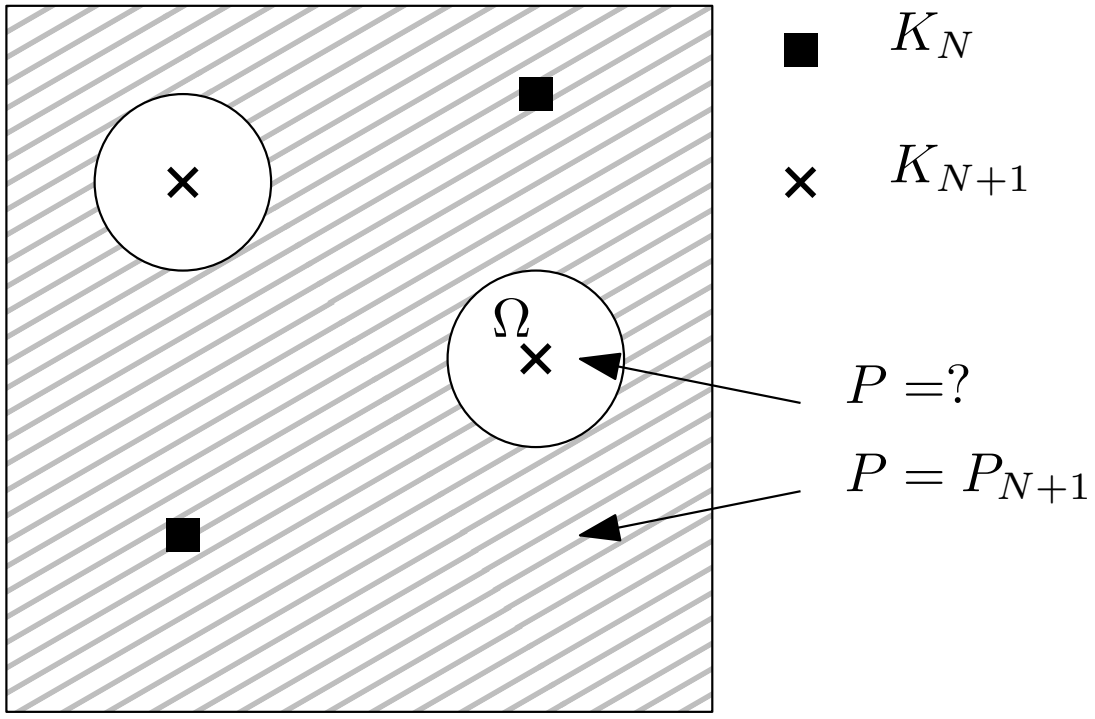
$$v(k) = \frac{rv(\omega) + (1-r)v^*}{|rv(\omega) + (1-r)v^*|}$$

□

General proof by induction on Rank P

Back to our problem

We can only continue P_{N+1} inside Ω when $Ch(P_{N+1}, \partial\Omega) = 0$, which is not the case at crossings



Impossible to continue P

Back to our problem

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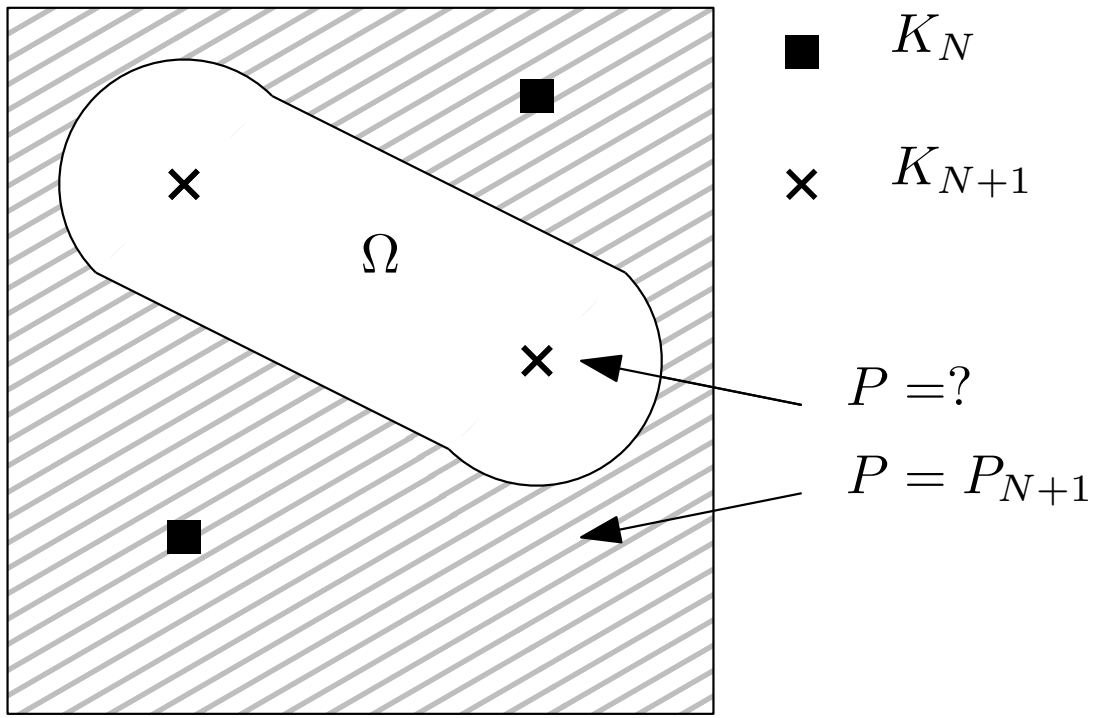


Solution: group the crossings to cancel Weyl charge

Then, $Ch(P_{N+1}, \partial\Omega) = -\frac{1}{2\pi}\int_{\Omega^c} d\mathcal{F}(P_{N+1}) = 0$ because P_{N+1} is well-defined outside of Ω, and so P_{N+1} can be extended to Ω.
It remains to make sure that $\mathrm{Ran}\, P_N \subset \mathrm{Ran}\, P_{N+1}$ on Ω (not shown but possible because P_N also has Chern 0). □

Difficulties and extensions

- We've built P, we now need to make sure we can find a basis of it: do the construction while respecting time-reversal symmetry
- Need to be careful when the crossing sets are lines, and when they are at time-reversal invariant points
- Can we also impose that $\operatorname{Ran} P \subset \operatorname{Ran} P_{N+2}$? Yes, if K_{N+2} is composed of points and curves, and $K_{N+1} \cap K_{N+2} = \emptyset$
- Can we do this with analytic functions (push from almost-exponential to exponential localization)? No, because P and all its derivatives have to match with P_N on K_N!

- What do we do in practice?

The Marzari-Vanderbilt scheme for insulators

Want to reproduce bands $1, \ldots, N$ by computing N Wannier functions

- At each point in the discretized Brillouin zone, solve $H(k)$ for its eigenvectors $u_n(k)$, $n = 1, \ldots, N$
- Let $v_n(k) = \sum_{n=1}^{N} u_m(k) U_{mn}(k)$, where $U(k)$ is unitary
- Optimize smoothness of $v_n(k)$ with respect to $U(k)$
- Reconstruct $\widetilde{H}_{mn}(k) = \langle v_m(k), H(k) v_n(k) \rangle$
- Interpolate $\widetilde{H}_{mn}(k)$ to a finer grid
- Diagonalize $\widetilde{H}_{mn}(k)$ on the finer grid

The Souza-Marzari-Vanderbilt scheme for metals

Want to reproduce bands $1, \ldots, N_f$ (frozen window) by computing N_w Wannier functions in the span of the first N_o bands (outer window)

- At each point in the discretized Brillouin zone, solve $H(k)$ for its eigenvectors $u_n(k)$, $n = 1, \ldots, N_o$
- Let $v_n(k) = \sum_{n=1}^{N_o} u_m(k) U_{mn}(k)$ for $n = 1, \ldots, N_w$, where $U(k)$ has orthogonal columns
- Optimize smoothness of $v_n(k)$ with respect to $U(k)$
- Reconstruct $\widetilde{H}_{mn}(k) = \langle v_m(k), H(k) v_n(k) \rangle$
- Interpolate $\widetilde{H}_{mn}(k)$ to a finer grid
- Diagonalize $\widetilde{H}_{mn}(k)$ on the finer grid

How to ensure that bands $1, \ldots, N_f$ are reproduced exactly?

Minimization of the MV functional for metals

- Souza-Marzari-Vanderbilt scheme: $\Omega = \Omega_I + \widetilde{\Omega}$, where Ω_I depends only on the space spanned by the WF (*gauge-independent*).
  1. Minimize Ω_I by a self-consistent procedure on UU^*
  2. Minimize $\widetilde{\Omega}$ as in the isolated case

  This is suboptimal because it does **not** minimize Ω.
- Combined scheme [Thygesen/Hansen/Jacobsen '05], [Damle/Levitt/Lin '18]:

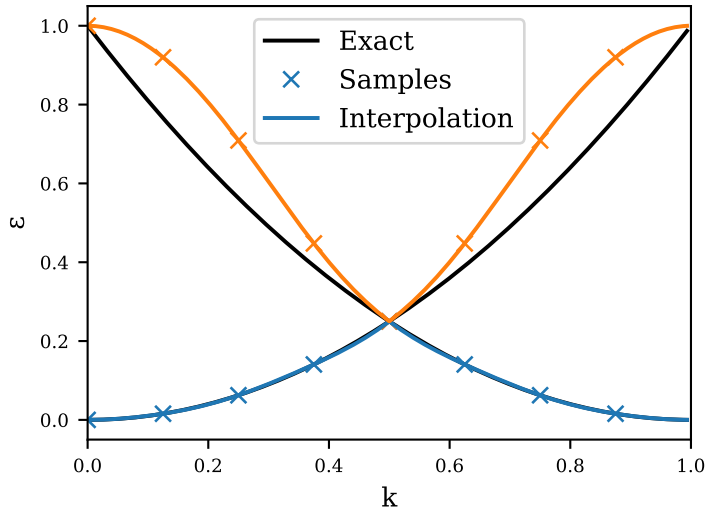
$$U(k) = \begin{pmatrix} I_{N_f} & 0 \\ 0 & Y(k) \end{pmatrix} X(k)$$

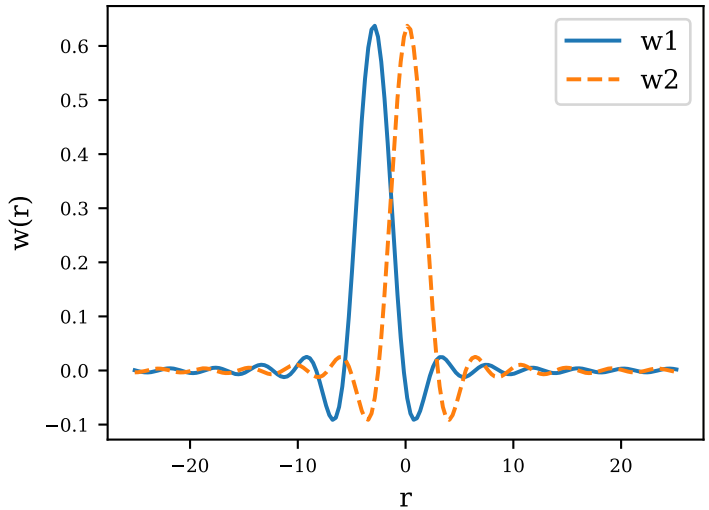
  where X is $N_w \times N_w$ unitary, and Y is $(N_o - N_f) \times (N_w - N_f)$ with orthogonal columns.
- Redundant but convenient for optimization: can be minimized by standard methods for optimization under orthogonality constraints (LBFGS on the Stiefel manifold: `Optim.jl` Julia library)
- More robust and efficient than SMV/`Wannier90` scheme, results more compact (but qualitatively similar)
- Initial guess: SCDM on a pseudo-density matrix [Damle/Lin '17]

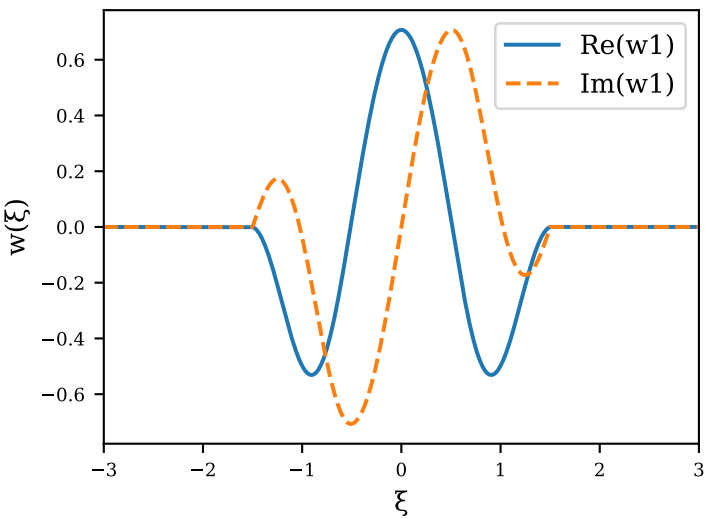
code online: `https://github.com/antoine-levitt/wannier` `https://github.com/asdamle/SCDM`

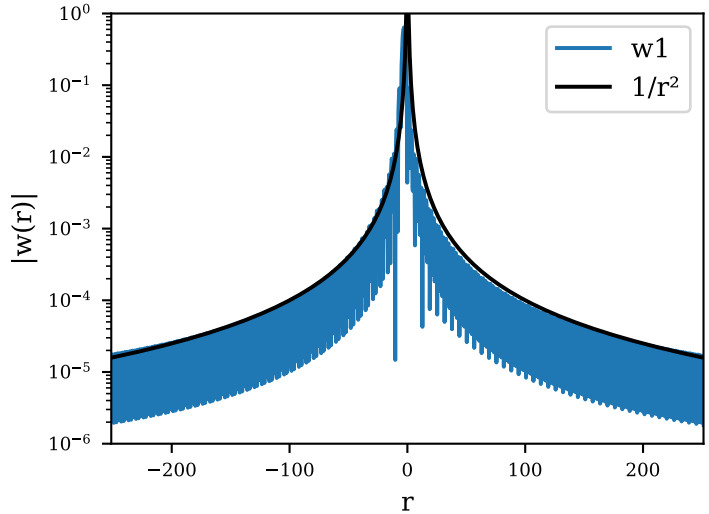
Decay properties of Wannier functions

Simple (but highly non-generic) model: free electron gas. Two Wannier functions spanning the first band





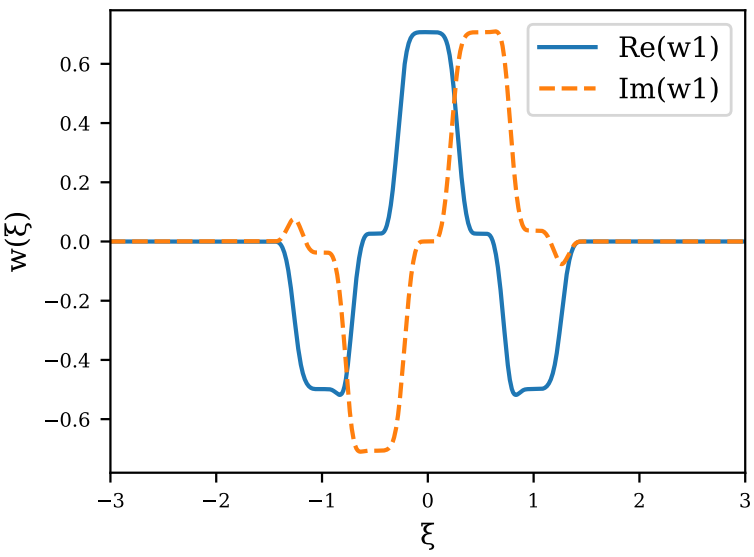


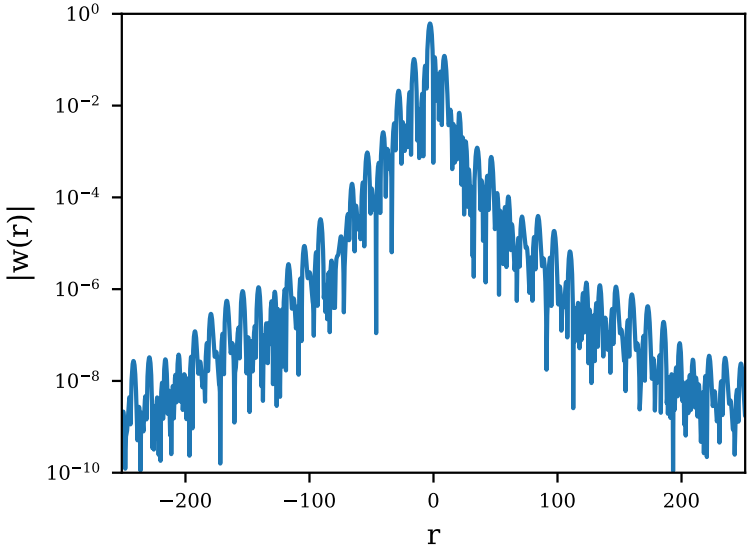


sinc-like quadratically decaying shift-orthogonal basis of bandlimited functions

Decay properties of Wannier functions

- Analogous results in 2D: decay as r^{-2}, in contrast to the isolated case (exponential decay, cf [Panati/Pisante '11])
- The discontinuous constraints $\operatorname{Ran} P_N \subset \operatorname{Ran} P$ prevent better regularity than that imposed explicitly by the functional
  pulling on a rope smoothens it, but if you hold one point there is a kink
- Can be fixed in an ad-hoc way for this system with cutoff functions:





Almost-exponentially localized shift-orthogonal basis of bandlimited functions

Conclusion and perspectives

- Isolated band structure: clear theory, efficient and robust algorithms
- Disentangled band structure
  - Almost-exponentially localized Wannier functions exist [Cornean/Gontier/Levitt/Monaco '18]...
  - ... but maximally-localized Wannier functions are only algebraically localized [Damle/Levitt/Lin '18]
  - Robust algorithms

Perspectives

- Weyl semimetals, $\mathbb{Z}_2$ topological insulators?
- How to find WF that are localized asymptotically as well as pre-asymptotically?
- Beyond Wannier interpolation?