Localised Wannier functions in metallic systems

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Joint work with H. Cornean, A. Levitt, D. Monaco.

Wannier functions

- Introduced by Wannier in 1937[1].
- $\equiv$ localised basis for periodic Schrödinger operators.
- Used for the study of crystals:
  - **theory:** modern theory of polarisation
  - **practice:** speed up calculations, construction of tight-binding models,...
  - **visualisation:** Wannier function $\sim$ location of electrons in crystals.

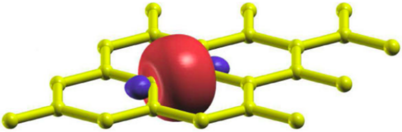


Figure: A localised Wannier function[2].

[1] G.H. Wannier, *Phys. Rev.* 52.3 (1937).

[2] from N. Marzari *et al.*, *Rev. Mod. Phys.* 84 (2012).

Statement of the problem (up to a Bloch transform -see later)

Let $\mathbb{T}^d \ni \mathbf{k} \mapsto H(\mathbf{k})$ be a smooth family of compact resolvent operators acting on $\mathbb{C}^M$.
$M \in \mathbb{N} \cup \{\infty\}$ and $\mathbb{T}^d$ is the d-dimensional torus.

$$H(\mathbf{k}) = \sum_{n=1}^{M} \varepsilon_{n\mathbf{k}} |u_{n\mathbf{k}}\rangle\langle u_{n\mathbf{k}}|, \quad \varepsilon_{1\mathbf{k}} \le \varepsilon_{2\mathbf{k}} \le \cdots, \quad (u_{n\mathbf{k}})_{n \le M} \text{ orthonormal basis of } \mathbb{C}^M.$$

Band crossing locations: $K_n := \left\{ \mathbf{k} \in \mathbb{T}^d, \ \varepsilon_{n\mathbf{k}} = \varepsilon_{n+1,\mathbf{k}} \right\}$.

Projection on the N lowest occupied states:

$$\forall \mathbf{k} \in \mathbb{T}^d \setminus K_N, \quad P_N(\mathbf{k}) = \sum_{n=1}^{N} |u_{n\mathbf{k}}\rangle\langle u_{n\mathbf{k}}| \quad \left(= \oint_{\mathscr{C}} \frac{\mathrm{d}z}{z - H(\mathbf{k})} \right).$$

Example: if $K_N = \emptyset$, then $P_N(\mathbf{k})$ is smooth and periodic (Insulating case).

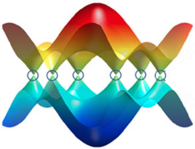
Wannier functions for insulators

Assume there exists $N \ll M$ such that $K_N = \emptyset$. Can we find a smooth and periodic family of N orthogonal functions (= frame)

$$\Psi(\mathbf{k}) := (\psi_1(\mathbf{k}), \cdots, \psi_N(\mathbf{k})) \in (\mathbb{C}^M)^N$$

such that $\mathrm{Ran}\, P_N(\mathbf{k}) = \mathrm{Span}\{\Psi(\mathbf{k})\}$.

Remark: For $d \ge 2$, the functions $\mathbf{k} \mapsto u_{n\mathbf{k}}$ **are not** smooth in general (conical band crossings).



Assume Wannier functions exist...

Reduced model: $\tilde{H}(\mathbf{k})$ of size $N \times N$, with

$$[\tilde{H}(\mathbf{k})]_{i,j} := \langle \psi_i(\mathbf{k}), H(\mathbf{k})\psi_j(\mathbf{k}) \rangle.$$

The matrix $\tilde{H}(\mathbf{k})$ is smooth and periodic, of size $N \times N$ with $N \ll M$, and its spectrum is exactly the lowest part of the spectrum of $H(\mathbf{k})$.

$\implies$ Can be used to speed numerical computations!

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In the framework of condensed matter physics. Periodic Schrödinger operators

$$H := -\Delta + V_{\text{per}} \quad = \int_{\mathbb{T}^d}^{\oplus} H(\mathbf{k}) \mathrm{d}\mathbf{k} \quad \text{(Bloch transform)}.$$

where $H(\mathbf{k}) := (-\mathrm{i}\nabla + \mathbf{k})^2 + V_{\text{per}}$ is smooth in $\mathbf{k}$ and (quasi-)periodic.

Wannier functions

If $\mathbb{T}^d \ni \mathbf{k} \mapsto \psi_n(\mathbf{k}) := \psi_n(\mathbf{k}, \mathbf{r})$ is smooth and periodic, then

$$w_n(\mathbf{r}) := \int_{\mathbb{T}^d} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}} \psi_n(\mathbf{k}, \mathbf{r}) \mathrm{d}\mathbf{k} \quad \text{is a localised Wannier function.}$$

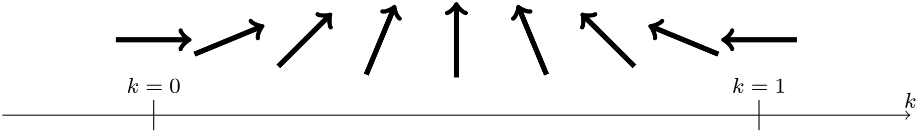
Wannier functions for insulators

Assume $P_N(\mathbf{k})$ smooth and periodic. Can we find a smooth and periodic frame

$$\Psi(\mathbf{k}) := (\psi_1(\mathbf{k}), \cdots, \psi_N(\mathbf{k})) \in (\mathbb{C}^M)^N$$

such that $\mathrm{Ran}\, P_N(\mathbf{k}) = \mathrm{Span}\{\Psi(\mathbf{k})\}$.

Topological obstruction



Theorem (G. Panati, *Ann. Henri Poincaré*, 8-5 (2007))

For all $d \leq 3$, if $P(\mathbf{k})$ is time-reversal symmetric (TRS), i.e. $P(-\mathbf{k}) = KP(\mathbf{k})K$, where K is the complex conjugation operator, then we can always construct a smooth periodic frame Ψ for P.

Works for periodic Schrödinger operators with *real-valued* potentials.

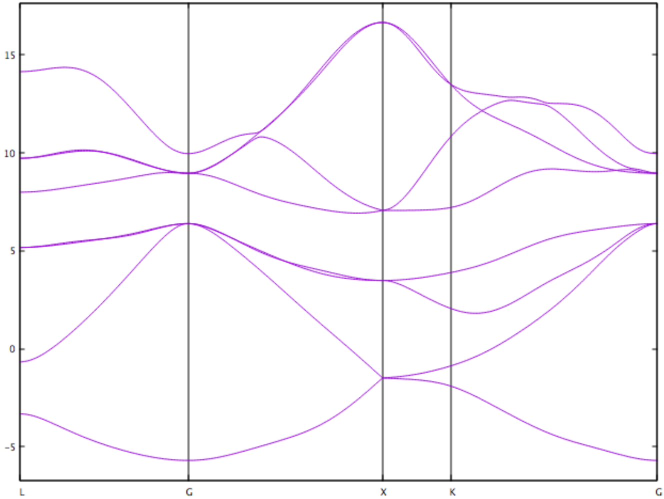


Figure: 8 first eigenvalues of silicon.

[2] Courtesy of S. Siraj-Dine, with the Wannier90 software.

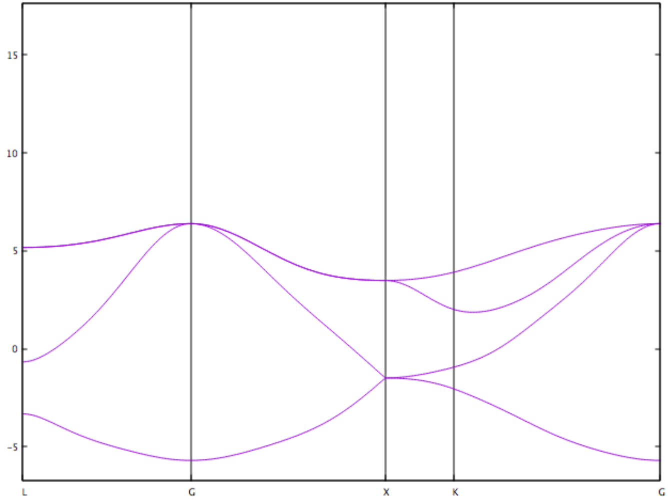


Figure: reduced model: 4 first eigenvalues of silicon computed on a $4 \times 4 \times 4$ grid $\subset \mathbb{T}^3$.

[2]Courtesy of S. Siraj-Dine, with the Wannier90 software.

What about metallic systems (no gap condition)? P_N is only defined on $\mathbb{T}^d \setminus K_N$...

Wannier functions for metals

Can we find a smooth projector $P(\mathbf{k})$ of rank $N+1$ such that $P_N(\mathbf{k}) \subset P(\mathbf{k})$ on $\mathbb{T}^d \setminus K_N$?

Remark: If $K_{N+1} = \emptyset$, then we can take $P = P_{N+1}$.

Theorem (H. Cornean, DG, A. Levitt, D. Monaco, arXiv 1712.07954)

Assume $d = 3$, that K_N and K_{N+1} are unions of points and piecewise smooth curves, and that $K_N \cap K_{N+1} = \emptyset$. Then we can find a such a smooth projection P.

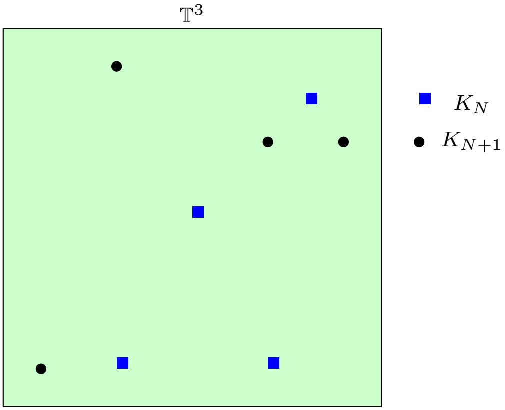
In addition, if P_N is TRS, then we can choose P to be TRS as well

Remarks

- These assumptions are met for most real-life systems.
- In the TRS case, according to the previous theorem, we can build a smooth periodic frame Ψ for P, of size $(N+1)$, and $\mathrm{Ran}\, P_N(\mathbf{k}) \subset \mathrm{Span}\{\Psi(\mathbf{k})\}$.

$\Longrightarrow$ We obtain a reduced model $\tilde{H}(\mathbf{k})$ of size $(N+1) \times (N+1)$, whose N lowest eigenvalues of are exactly the N lowest eigenvalues of $H(\mathbf{k})$.

Flavour of the proof



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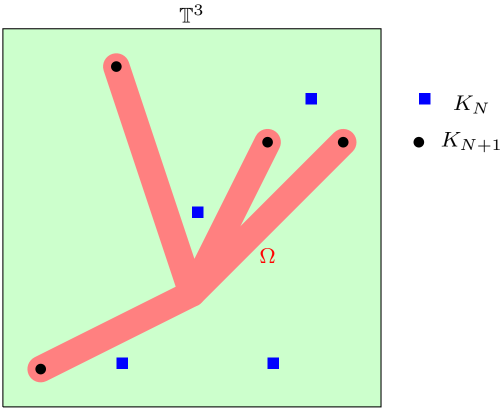

- The set Ω is chosen such that $K_{N+1} \subset \Omega$, $K_N \subset \mathbb{T}^3 \setminus \Omega$, and Ω is diffeomorphic to the ball $\mathbb{D}_3$.

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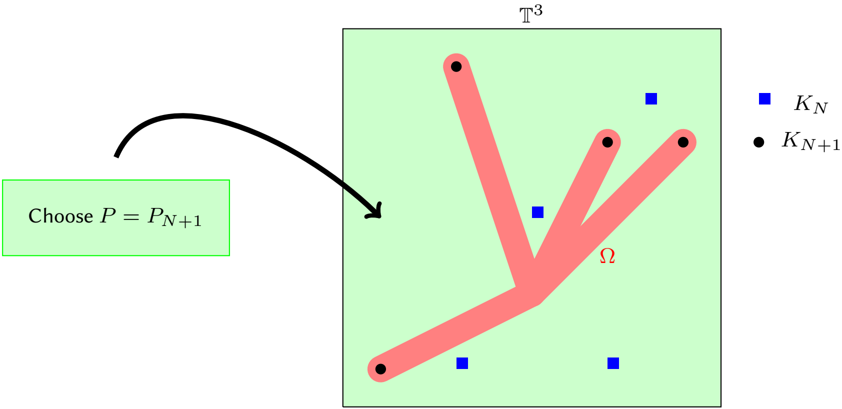

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- Choose $P = P_{N+1}$ on $\mathbb{T}^3 \setminus \Omega$

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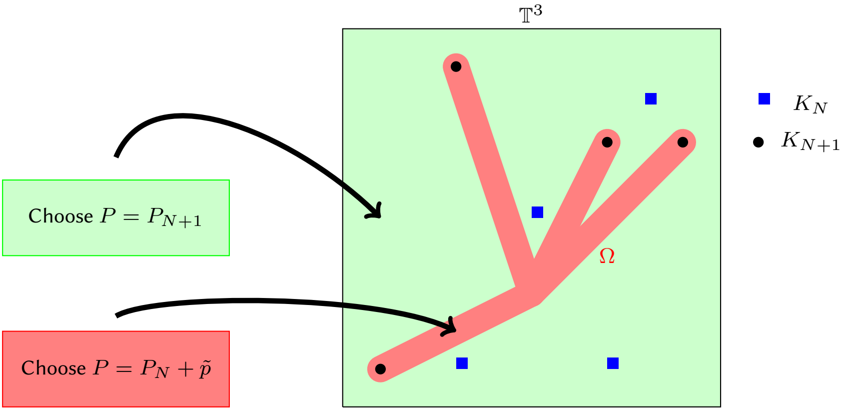

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- Choose $P = P_{N+1}$ on $\mathbb{T}^3 \setminus \Omega$, and choose $P = P_N + \tilde{p}$ on Ω.

Flavour of the proof

Choose $P = P_{N+1}$

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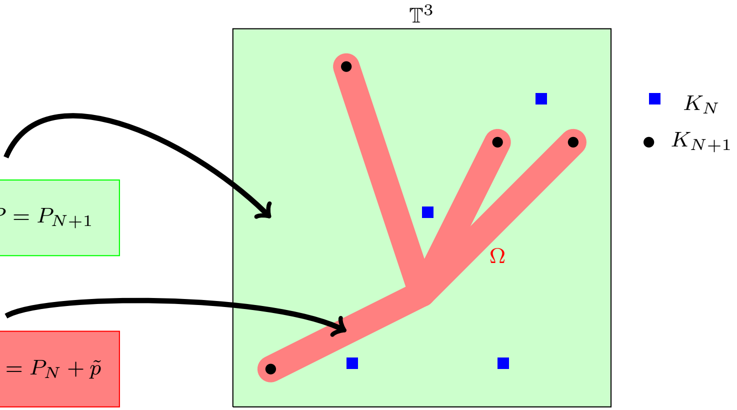

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$\Longrightarrow$ **Find a rank-1 projector** $\tilde{p} \in \Omega \sim \mathbb{D}_3$ **with** $\tilde{p} = P_{N+1} - P_N$ **on** $\partial\Omega \sim \mathbb{S}^2$**.**

Lemma

Let $P(\omega)$ be a smooth family of projectors defined on $\omega \in \mathbb{S}^2$.
There exists a smooth extension of P on $\mathbb{D}^3$ if and only if the Chern number $\mathrm{Ch}(P, \mathbb{S}^2)$ vanishes, where

$$\mathrm{Ch}(P, \mathbb{S}^2) := \frac{1}{2\mathrm{i}\pi} \int_{\mathbb{S}^2} \mathrm{Tr}\left(P \, \mathrm{d}P \wedge \mathrm{d}P\right).$$

In our case, $\tilde{p} = P_{N+1} - P$ on $\partial\Omega$, which implies

$$\mathrm{Ch}(\tilde{p}, \partial\Omega) = \mathrm{Ch}(P_{N+1}, \partial\Omega) - \mathrm{Ch}(P_N, \partial\Omega).$$

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We conclude that[3] $\mathrm{Ch}(\tilde{p}, \partial\Omega) = 0$, and that $\tilde{p}$ has a smooth extension on Ω.

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Thank you for your attention!

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