Maximally localized Wannier functions
for periodic Schrödinger operators:
the MV functional and the geometry of the Bloch bundle

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Bloch orbitals

The electronic ground state of a **periodic system** is usually described in terms of **Bloch orbitals**, *i. e.* simultaneous generalized eigenfunctions of the **periodic 1-particle Hamiltonian**

$$H_{\text{per}} = -\Delta + V_\Gamma$$

where

$$V_\Gamma(x+\gamma) = V_\Gamma(x), \qquad \text{for all } \gamma \in \Gamma = \text{Span}_{\mathbb{Z}}(e_1, \ldots, e_d) \cong \mathbb{Z}^d,$$

and of the **lattice translations** $\{T_\gamma\}_{\gamma\in\Gamma}$

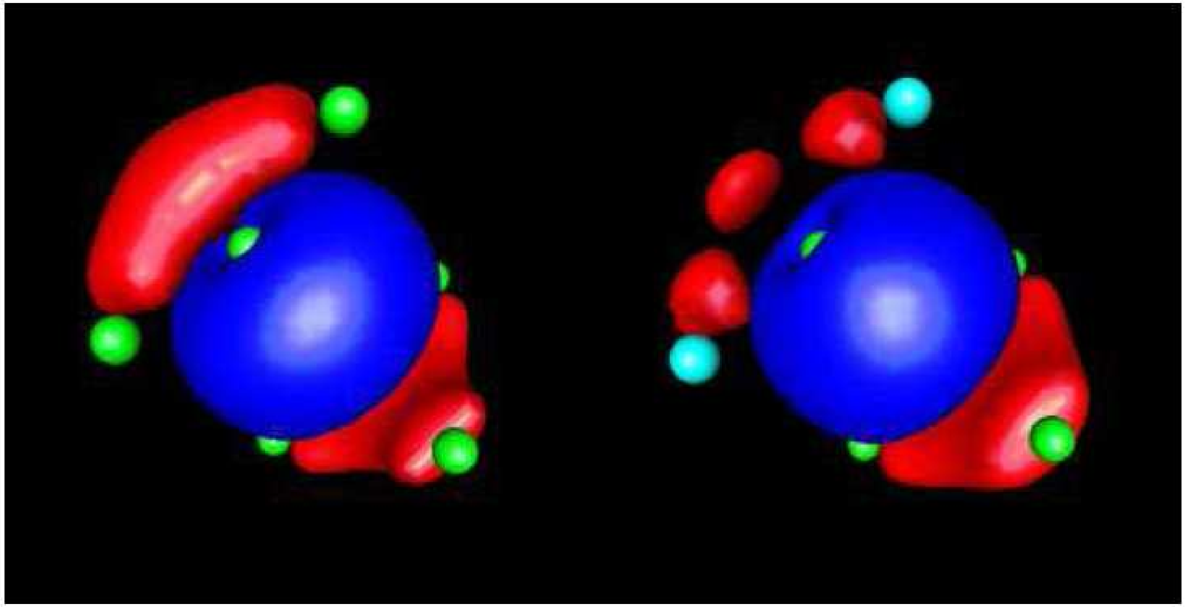
$$(T_\gamma \psi)(x) = \psi(x-\gamma).$$

While convenient for many purposes, these "orbitals" (= generalized eigenfunctions) have the disadvantage that are **not localized in position space.**

. . . and Wannier orbitals

An alternative representation in terms of **localized orbitals** has been introduced by **Gregory Wannier** in 1937. The main advantage of this approach is that Wannier functions are **localized in position space**. Thus

(i) they provide an intuitive (visual) insight into the **structure of chemical bonds** in crystals



Amplitude **isosurface contours** for maximally-localized Wannier functions in **Si** (left panel) and **GaAs** (right panel). Red and blue contours are for isosurfaces of identical absolute value but opposite signs; Si and As atoms are in green, Ga in cyan. Notice that **breaking of inversion symmetry** in GaAs polarizes the WFs towards the more electronegative As anion.

(Courtesy of N. Marzari, I. Souza and D. Vanderbilt)

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(i) they provide an intuitive (visual) insight into the **structure of chemical bonds** in crystals

(ii) in computational physics, localized Wannier functions are crucial to develop **numerical methods whose cost scales linearly** with the size of the confining box **[Gödecker]**

(iii) they are crucial in the **theory of polarization** of crystalline solids **[King-Smith & Vanderbilt, Resta]** and of **orbital magnetization** **[Ceresoli & Resta, Thonhauser & Vanderbilt]**.

All these advantages rely on the assumption that Wannier functions are indeed **exponentially localized.**

Is this always the case? Is there an alghoritm to obtain them?

For **constant coefficients** differential operators one introduces the Fourier transform, which yields the duality

Position space	$\longleftrightarrow$	**Momentum space**
Dirac's deltas $\{x \mapsto \delta_a(x)\}_{a \in \mathbb{R}^d}$	$\longleftrightarrow$	**Plane waves** $\{k \mapsto e^{ik \cdot a}\}_{a \in \mathbb{R}^d}$

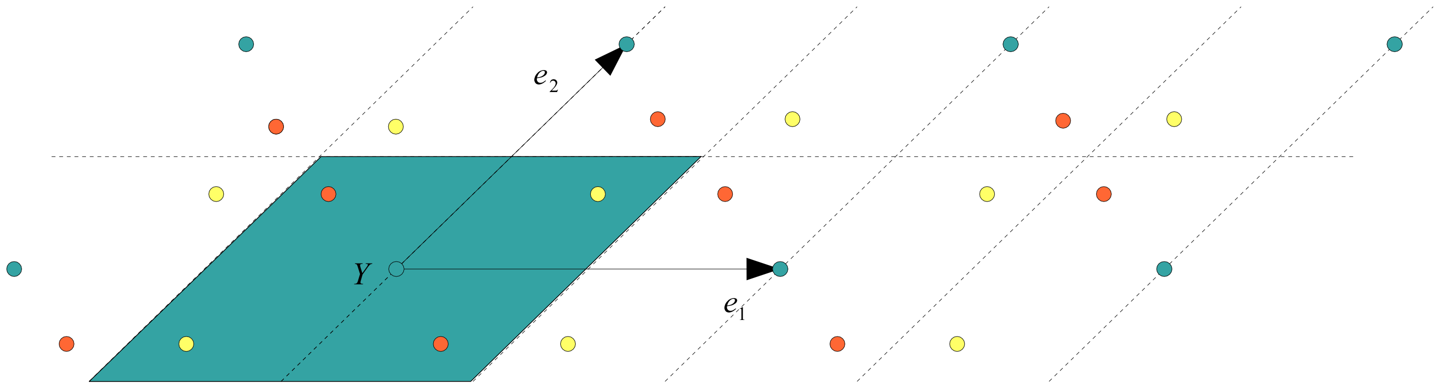
As far as differential operators with **periodic coefficients** are concerned

Position space	$\longleftrightarrow$	**Momentum space**
Wannier functions $\{x \mapsto w_{n,\gamma}(x)\}_{n \in \mathbb{N}, \gamma \in \Gamma}$	$\longleftrightarrow$	**Bloch waves** $\{k \mapsto \psi_n(k, \cdot)\}_{n \in \mathbb{N}}$

I
Periodic systems and

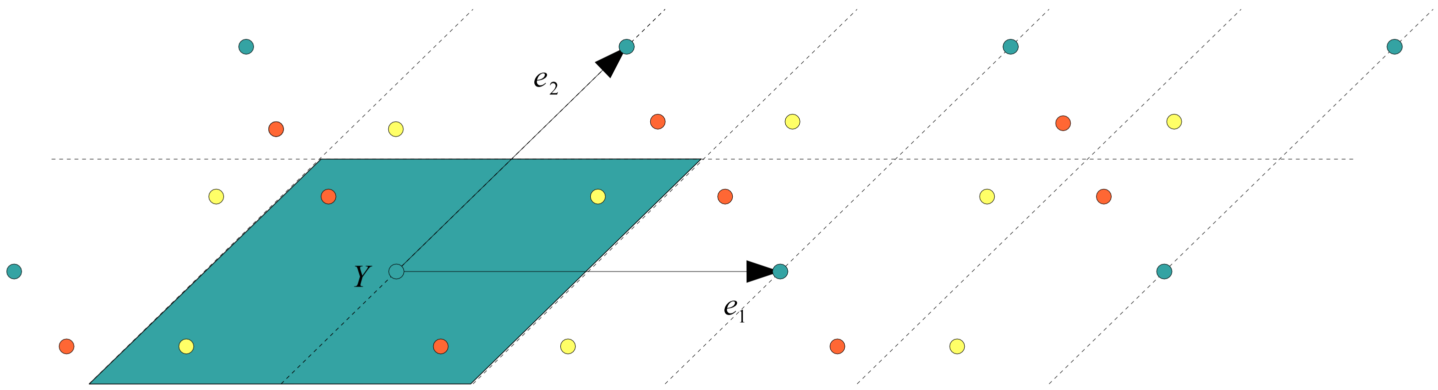
Bloch-Floquet transform

The **Bloch-Floquet** transform



	Configuration space	Momentum space
Lattice	Γ	Γ^*
Fundamental domain	Y	$\mathbb{B}$
	$\mathbb{T}_Y^d = \mathbb{R}^d/\Gamma$	$\mathbb{T}_d^* = \hat{\mathbb{R}}^d/\Gamma^*$
Hilbert space	$\mathcal{H}_{\mathrm{f}} = L^2(Y)$	

The **Bloch-Floquet** transform

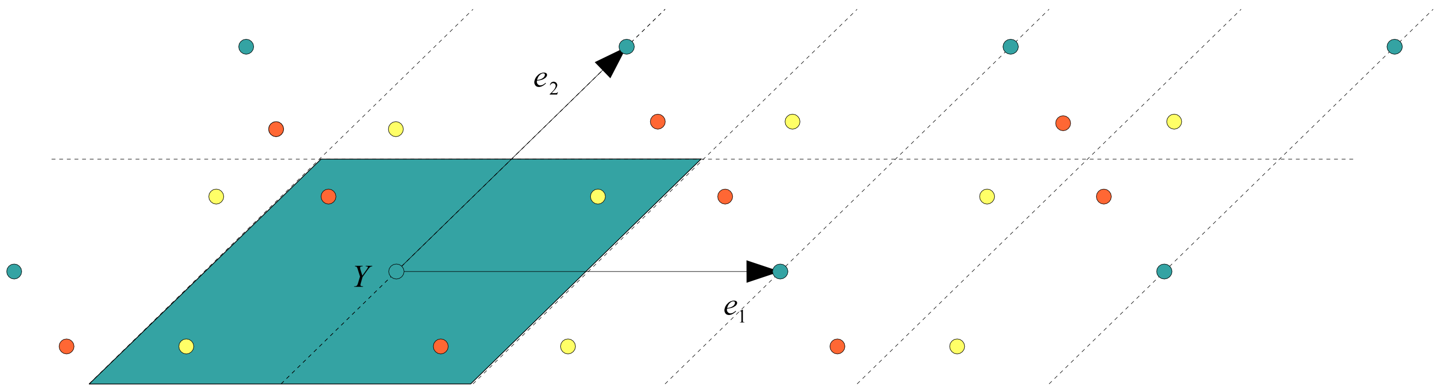


Assumption on V_Γ: we make the following **Kato-type assumption** on the Γ-periodic potential:

$$V_\Gamma \in L^2_{\mathrm{loc}}(\mathbb{R}^d) \text{ for } d \leq 3, \qquad V_\Gamma \in L^p_{\mathrm{loc}}(\mathbb{R}^d) \text{ with } p > d/2 \text{ for } d \geq 4,$$

to assure that $H = -\Delta + V_\Gamma$ is self-adjoint in $L^2(\mathbb{R}^d)$ on the domain $W^{2,2}(\mathbb{R}^d)$.

The Bloch-Floquet transform

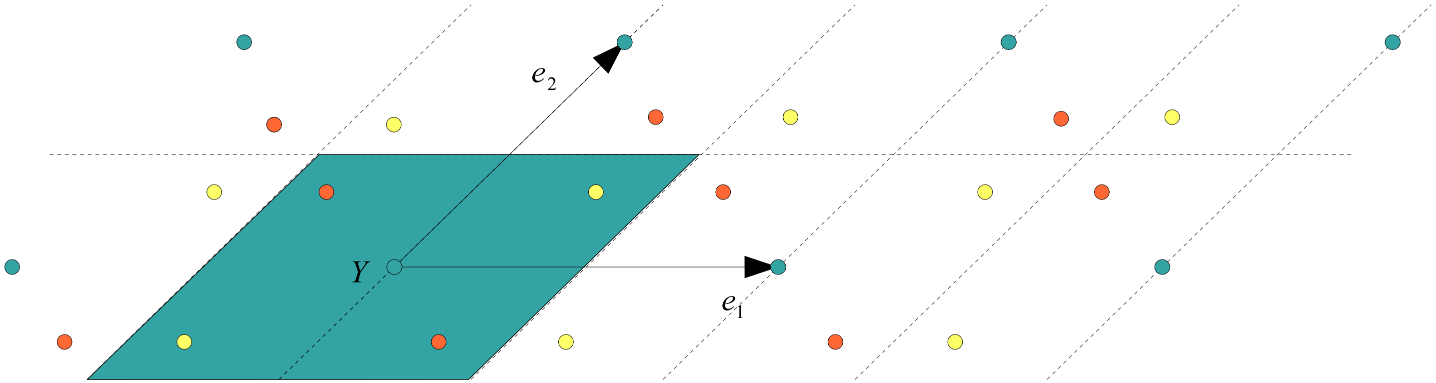


The **modified** Bloch-Floquet transform is defined as

$$\widetilde{\mathcal{U}} : L^2(\mathbb{R}^d) \longrightarrow L^2(\mathbb{B}) \otimes \underbrace{L^2(\mathbb{T}^d_Y)}_{\mathcal{H}_{\mathrm{f}}}$$

$$(\widetilde{\mathcal{U}}\psi)(k, y) = \frac{1}{|\mathbb{B}|^{1/2}} \sum_{\gamma \in \Gamma} \mathrm{e}^{-i(y+\gamma)\cdot k} \; \psi(y+\gamma), \quad k, y \in \mathbb{R}^d.$$

The **Bloch-Floquet** transform



Notice that

$$(\widetilde{\mathcal{U}}\psi)(k + \lambda, y) = \mathrm{e}^{-iy\cdot\lambda}(\widetilde{\mathcal{U}}\psi)(k, y) \qquad \forall\lambda \in \Gamma^*$$

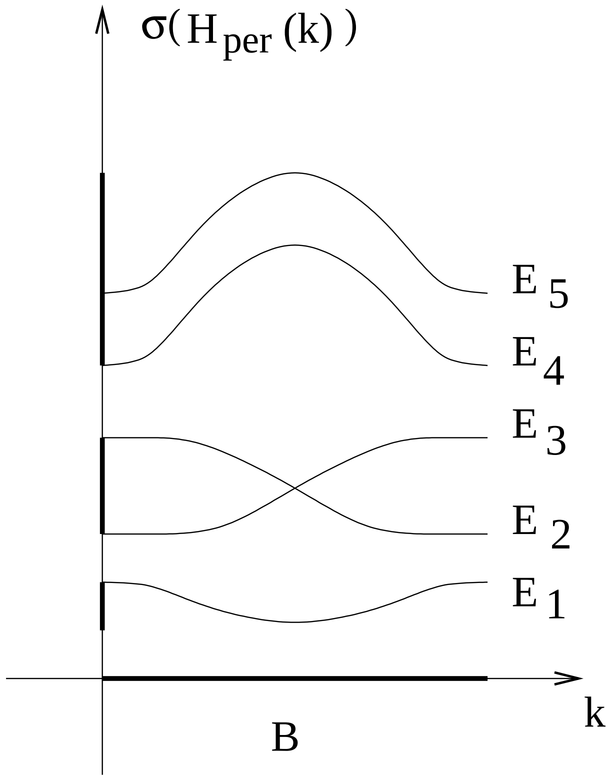
so that the transformed function is determined by the values assumed on $k \in \mathbb{B}$.

In modified BF representation $H = -\Delta + V_\Gamma$ becomes a **fibered operator**

$$\widetilde{\mathcal{U}}\, H\, \widetilde{\mathcal{U}}^{-1} = \int_{\mathbb{B}}^{\oplus} H_{\rm per}(k)\, dk \qquad \text{in } L^2(\mathbb{B}, \mathcal{H}_{\rm f}) \cong L^2(\mathbb{B}) \otimes \mathcal{H}_{\rm f},$$

$$H_{\rm per}(k) = \tfrac{1}{2}(-i\nabla_y + k)^2 + V_\Gamma(y) \qquad \text{acting on } \mathcal{D} = W^{2,2}(\mathbb{T}_Y^d) \subseteq L^2(\mathbb{T}_Y^d) = \mathcal{H}_{\rm f}\,.$$

The band structure:



Solution of the **eigenvalue problem**:

$$H_{\rm per}(k)\varphi_n(k,y) = E_n(k)\varphi_n(k,y)$$

Eigenvalue: $E_n(k)$

Eigenvector: $\varphi_n(k,\cdot) \in \mathcal{H}_{\rm f} = L^2(\mathbb{T}_Y^d, dy)$

Eigenprojector: $P_n(k) = |\varphi_n(k)\rangle\langle\varphi_n(k)|$

Total projector: $P_n = \{P_n(k)\}_{k\in\mathbb{B}}$

Bloch function: $\varphi_n \in L^2(\mathbb{B}, \mathcal{H}_{\rm f})$

Definition. A (normalized) **Bloch function** corresponding to the nth Bloch band is any $\varphi_n \in L^2(\mathbb{B}, \mathcal{H}_{\mathrm{f}})$ such that

$$H_{\mathrm{per}}(k)\varphi_n(k,y) = E_n(k)\varphi_n(k,y) \qquad \|\varphi_n(k,\cdot)\|_{\mathcal{H}_{\mathrm{f}}} = 1 \qquad \text{for a.e. } k \in \mathbb{B}$$

$$\varphi_n(k+\lambda, y) = \mathrm{e}^{-iy\cdot\lambda}\,\varphi_n(k,y) \qquad \forall \lambda \in \Gamma^*, k \in \partial\mathbb{B}.$$

The last condition is called **equivariance** or **pseudoperiodicity**. It will become crucial when requiring some regularity on the map $k \mapsto \varphi_n(k,\cdot)$.

II
Wannier functions:
the isolated band case

Wannier functions and gauge freedom

Let φ_n be a Bloch function corresponding to an **isolated Bloch band** E_n. Notice that the choice of φ_n is **not unique**, since the function

$$\widetilde{\varphi}_n(k,y) = e^{i\vartheta(k)}\varphi_n(k,y)$$

is also an eigenfunction of $H_{\mathrm{per}}(k)$ corresponding to $E_n(k)$ (**Bloch gauge**).

Definition. The **Wannier function** $w_n \in L^2(\mathbb{R}^d)$ corresponding to a Bloch function φ_n is the preimage of φ_n by the Bloch-Floquet transform, *i. e.*

$$w_n(x) := \left(\widetilde{\mathcal{U}}^{-1}\varphi_n\right)(x) = \frac{1}{|\mathbb{B}|^{1/2}}\int_{\mathbb{B}} e^{ik\cdot x}\varphi_n(k,x)dk, \qquad x \in \mathbb{R}^d.$$

Note: it is misleading to talk about "the Wannier function for the nth band".

Some **elementary properties** of the Wannier functions:

(i) the **translated Wannier functions** are written as

$$w_{n,\gamma}(x) \equiv w_n(x-\gamma) = \frac{1}{|\mathbb{B}|^{1/2}} \int_{\mathbb{B}} e^{-ik\cdot\gamma} \varphi_n(k,x)\, dk, \qquad \gamma \in \Gamma.$$

(ii) if the norm $\|\varphi_n(k,\cdot)\|_{L^2(Y)}$ is k-independent, then the functions $\{w_{n,\gamma}\}_{\gamma\in\Gamma}$ are **mutually orthogonal** in $L^2(\mathbb{R}^d)$.

(iii) under this condition the family $\{w_{n,\gamma}\}_{\gamma\in\Gamma}$ is a **complete orthonormal basis of** $\operatorname{Ran} P_n$.

(iv) if $I_n := \operatorname{Ran} E_n \subset \mathbb{R}$ is **isolated from the rest of the spectrum** of H, then $\operatorname{Ran} P_n$ is the spectral projector of H corresponding to the interval $I_n \subset \mathbb{R}$.

Globally, the family of all Wannier functions $\{w_{n,\gamma}\}_{n\in\mathbb{N},\gamma\in\Gamma}$ is a **complete orthonormal basis** of $L^2(\mathbb{R}^d)$.

Question (A): to which extent are the Wannier functions **localized**?

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Localization in position space	$\longleftrightarrow$	**Smoothness in momentum space**

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Localization in position space	$\longleftrightarrow$	**Smoothness in momentum space**
Decay faster than any polynomial	$\longleftrightarrow$	**Infinite differentiability**
Decay faster than an exponential	$\longleftrightarrow$	**Analyticity in a complex strip**

Question (A$'$): how **smooth** is the Bloch function ?

The question is ill-posed, it crucially **depends on the choice of the phase**.

In numerical simulations the phase is random. Therefore one has to **readjust phases** *a posteriori* in order to obtain reasonably localized Wannier functions.

Question (A$''$): is it possible to **choose the phase (Bloch gauge)** of the eigenfunctions $\varphi_n(k, \cdot)$ so that the corresponding Wannier function is **exponentially localized**?

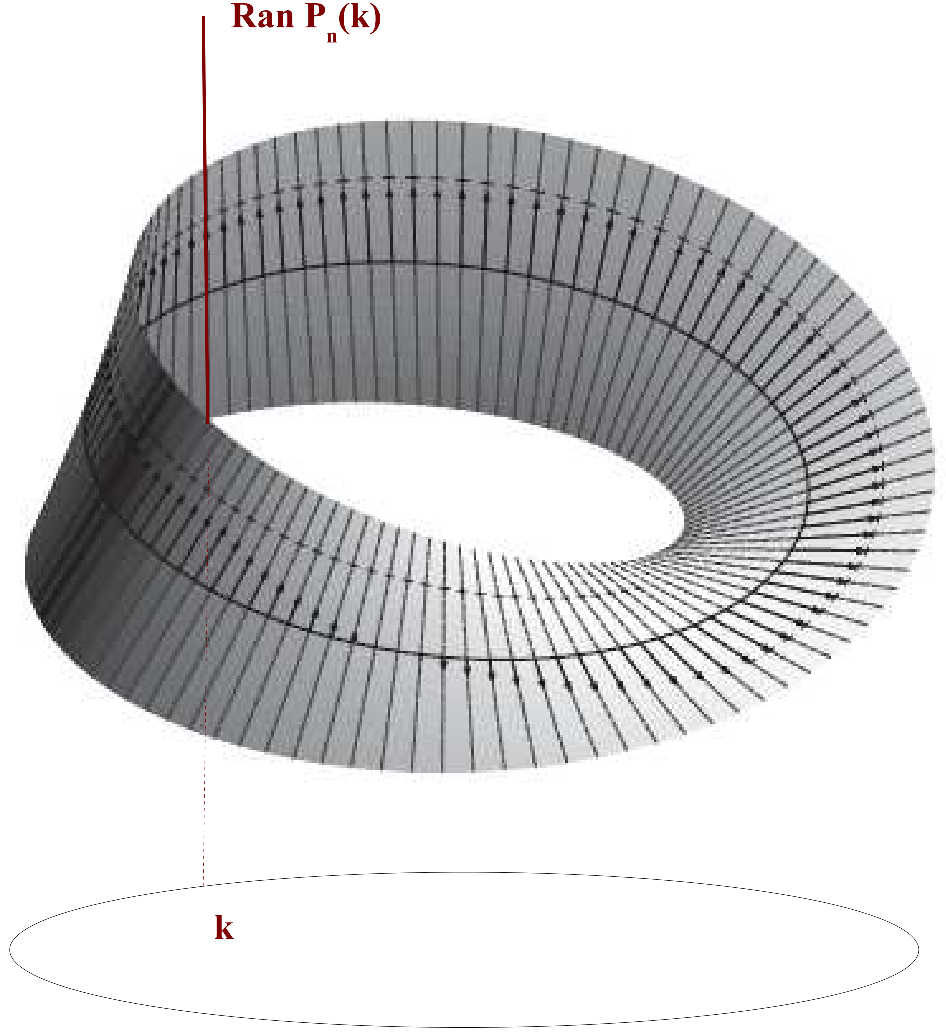
It seems very easy . . .

Since the band E_n is assumed to be an **isolated band** one has that

$$k \mapsto P_n(k) \quad \text{is smooth (even analytic in a complex strip } \Omega_\alpha \subset \mathbb{C}^d)$$

$$k \mapsto \varphi_n(k, \cdot) \quad \text{can be chosen } \textbf{locally smooth}$$

. . . but a topological obstruction might appear!!



Answer(A): the answer is positive for an **isolated Bloch band**.

$d = 1$	W. Kohn (1959)
$d > 1$	de Cloiseaux (1964) requiring **space-reflection symmetry**
$d > 1$	G. Nenciu (1983), B. Helffer & J. Sjöstrand (1989).

The result depends crucially on the fact that the Hamiltonian

$$H = -\Delta + V_\Gamma$$

is **real**, *i.e.* the system is **time-reversal symmetric (TR)**.

For a non TR-symmetric operator, *e.g.*

$$H_B = \frac{1}{2}\left(-i\nabla_x + A_B(x)\right)^2 + V_\Gamma,$$

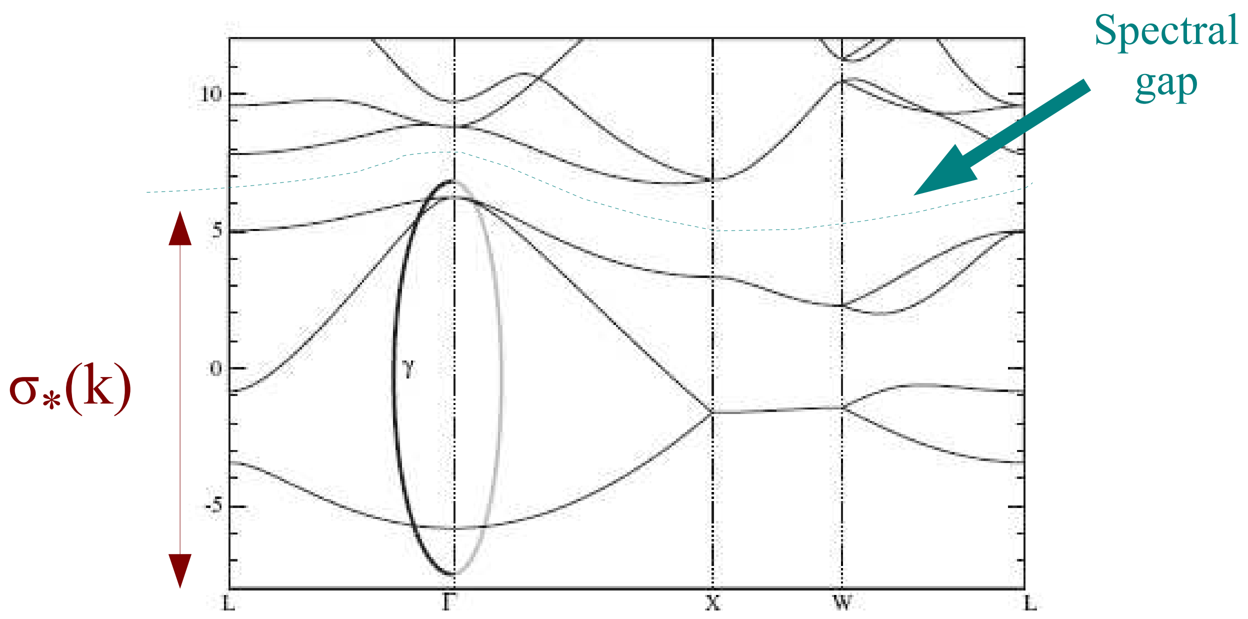
counterexamples appear already for $d = 2$. **[Dubrovin, Novikov, Lyskova]**.

On the other hand, in some cases one may recover the result by exploiting **magnetic TR symmetry** **[De Nittis & Lein]**.

III
Wannier functions:
the multi-band case

Eigenvalue crossings

In dimension $d = 3$ there are generically **no isolated Bloch bands**.



However, in insulators there is a **spectral gap**. Then it is interesting to consider the family of bands which are below the gap.

Let $\sigma_*(k) \subset \mathbb{R}$ be an interval including at every k the **relevant family of bands**.

The Bloch functions do **not** have a smooth continuation across the **crossing points** (except in dimension $d = 1$). Thus no hope to obtain directly exponentially localized Wannier functions.

Vision (de Cloiseaux): let us consider **the relevant family of bands as a unity.**

Let $P_*(k)$ be the orthogonal projector on the relevant family of bands, *i. e.*

$$P_*(k) = \sum_{\{n: E_n(k) \in \sigma_*(k)\}} |\varphi_n(k)\rangle\langle\varphi_n(k)|.$$

Definition. A function $k \mapsto \chi(k, \cdot) \in \mathcal{H}_{\mathrm{f}}$ is called a **quasi-Bloch function** [de Cloiseaux 64] if $\chi \in L^2(\mathbb{B}, \mathcal{H}_{\mathrm{f}})$

$$P_*(k)\chi(k, \cdot) = \chi(k, \cdot), \qquad \chi(k, \cdot) \neq 0 \qquad \text{for a.e. } k \in \mathbb{B}$$

and it is **Γ^*-equivariant**, *i. e.*

$$\chi(k + \lambda, y) = \mathrm{e}^{-iy\cdot\lambda}\, \chi(k, y) \qquad \forall \lambda \in \Gamma^*, k \in \partial\mathbb{B}.$$

Let $m := \dim \operatorname{Ran} P_*(k) < +\infty$.

Definition. A **Bloch frame** is a family $\{\chi_a\}_{a=1,\dots,m}$ of **quasi-Bloch functions** such that

$$\{\chi_1(k,\cdot),\dots,\chi_m(k,\cdot)\} \text{ is an } \textbf{orthonormal basis} \text{ of } \operatorname{Ran} P_*(k) \quad \forall k \in \mathbb{B}.$$

Definition. The **composite Wannier functions** corresponding to a Bloch frame $\{\chi_a\}_{a=1,\dots,m}$ are defined as

$$w_a(x) := \left(\widetilde{\mathcal{U}}^{-1}\chi_a\right)(x), \qquad a \in \{1,\dots,m\}.$$

Notice that the family $\{w_{a,\gamma}\}_{a=1,\dots,m;\gamma\in\Gamma}$ is an **orthonormal basis** of the spectral subspace corresponding to the energy window $\operatorname{Ran}\sigma_*$.

Composite Wannier functions and Bloch gauge

A Bloch frame is fixed only up to a k-dependent unitary matrix $U \in \mathcal{U}(\mathbb{C}^m)$, *i. e.*

$$\widetilde{\chi}_a(k) = \sum_{b=1}^{m} U_{a,b}(k)\chi_b(k)$$

is still a Bloch frame if $\{\chi_a\}_{a=1,\ldots,m}$ is a Bloch frame.

Question (B): is there a choice of **Bloch gauge** which makes the composite Wannier functions **exponentially localized ?**

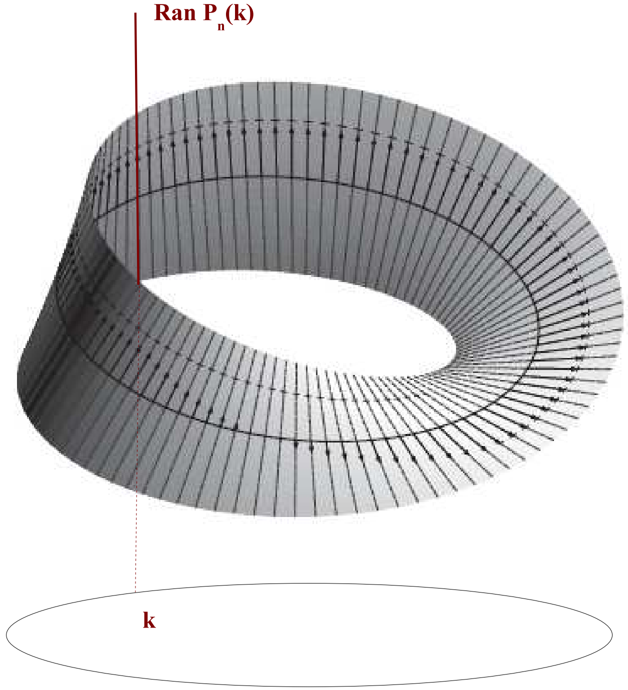
Question (B′): does exist a family of quasi-Bloch functions $k \mapsto \chi_a(k)$ such that

(B$_1$) each map $\chi_a : \mathbb{R}^d \longrightarrow \mathcal{H}_{\mathrm{f}}$ has a **analytic extension** to a strip;
(B$_2$) the set $\{\chi_1(k), \ldots, \chi_m(k)\}$ is an (orthonormal) basis **spanning** $\mathrm{Ran} P_*(k)$ for every $k \in \mathbb{B}$.

First answer to (B): yes for dimension $d = 1$ [G. Nenciu, 1983].

The **geometric** viewpoint

Vision: the problem is equivalent to a geometric one.

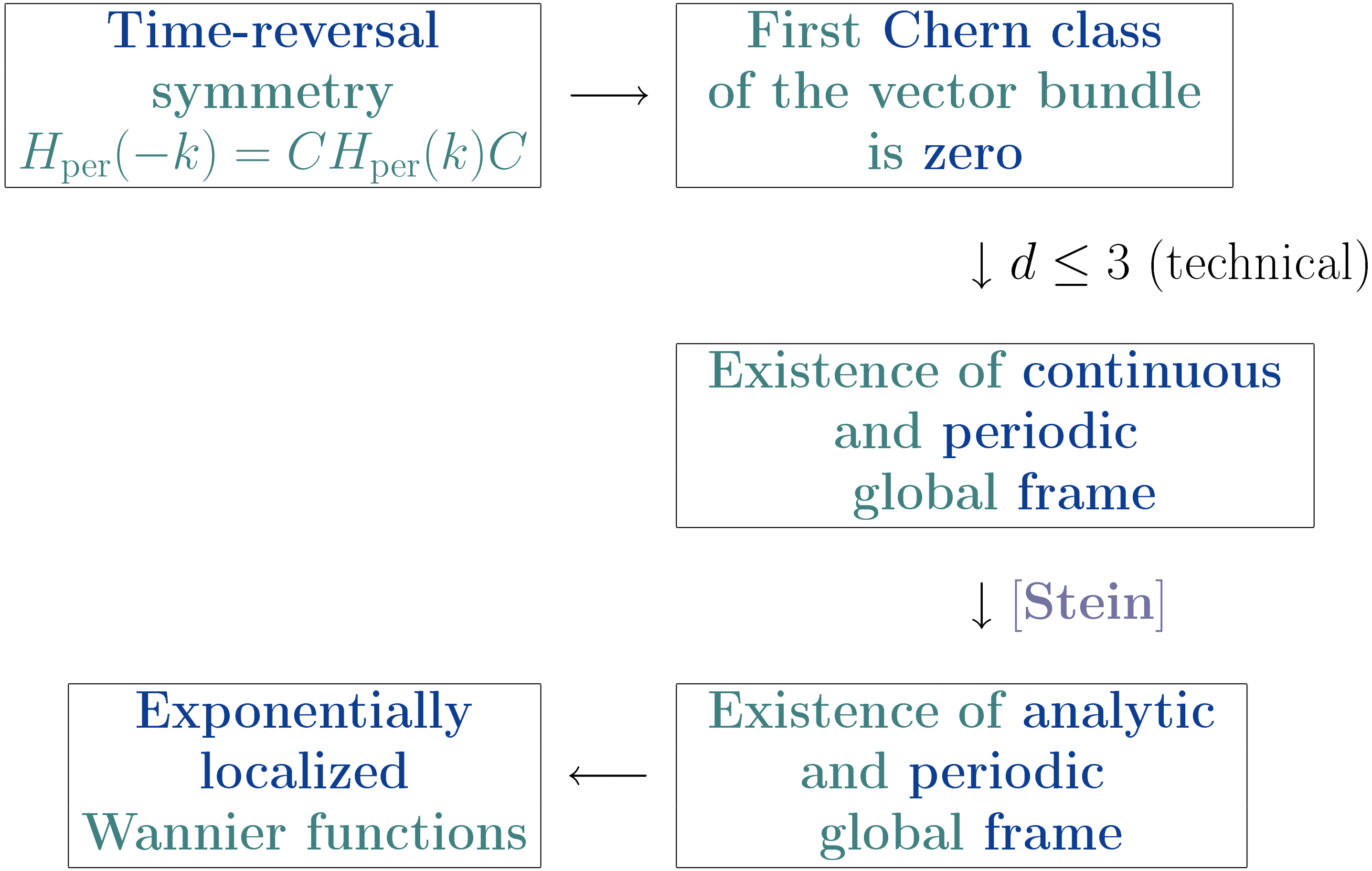


We are interested to prove the **triviality of a Hermitian vector bundle** over the d-dimensional torus $\mathbb{T}_d^*$.

The **geometric** viewpoint

Vision: the problem is equivalent to a geometric one. Moreover the **obstruction** might appear **only at the topological level**

Continuous solution $\overset{\text{Steenrod}}{\Longleftrightarrow}$ **Smooth solution** $\overset{\text{Stein}}{\Longleftrightarrow}$ **Analytic solution**



Time-reversal symmetry $H_{\text{per}}(-k) = C H_{\text{per}}(k) C$
First Chern class of the vector bundle is zero
$\downarrow d \leq 3$ (technical)
Existence of continuous and periodic global frame
$\downarrow$ [Stein]
Existence of analytic and periodic global frame
Exponentially localized Wannier functions

Second answer to (B): yes in dimension $d \leq 3$.

- G. Panati. *Triviality of Bloch and Bloch-Dirac bundles*, **Annales Henri Poincaré 8**, 995-1011 (2007).

- Ch. Brouder, G. Panati, M. Calandra, Ch. Mourougane and N. Marzari. *Exponential localization of Wannier functions in insulators*, **Phys. Rev. Lett. 98**, 046402 (2007).

PRL **98,** 046402 (2007) PHYSICAL REVIEW LETTERS week ending 26 JANUARY 2007

Exponential Localization of Wannier Functions in Insulators

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The exponential localization of Wannier functions in two or three dimensions is proven for all insulators that display time-reversal symmetry, settling a long-standing conjecture. Our proof relies on the equivalence between the existence of analytic quasi-Bloch functions and the nullity of the Chern numbers (or of the Hall current) for the system under consideration. The same equivalence implies that Chern insulators cannot display exponentially localized Wannier functions. An explicit condition for the reality of the Wannier functions is identified.

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IV
Maximally localized Wannier functions:
the Marzari-Vanderbilt functional

The Marzari-Vanderbilt localization functional

In the 90's, the long-lasting **uncertainty about the existence of exponentially localized composite WFs**, and the need of an approach suitable for **numerical simulations**, forced the solid state physics community to **change the perspective**:
one writes a convenient **localization functional** and look for its **minimizers** **[Marzari & Vanderbilt 97]**.

The Marzari-Vanderbilt localization functional

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one writes a convenient **localization functional** and look for its **minimizers** **[Marzari & Vanderbilt 97]**.

Definition For a single-band normalized Wannier function $w \in L^2(\mathbb{R}^d)$,

$$F_{MV}(w) := \sum_{j=1}^{d} \mathrm{Var}\left(X_j; |w(x)|^2 dx\right) = \int_{\mathbb{R}^d} |x|^2 |w(x)|^2 dx - \sum_{j=1}^{d} \left(\int_{\mathbb{R}^d} x_j |w(x)|^2 dx \right)^2,$$

which is well-defined at least whenever $\int_{\mathbb{R}^d} |x|^2 |w(x)|^2 dx < +\infty$.

More generally, for a system of L^2-normalized composite Wannier functions $w = \{w_1, \ldots, w_m\} \subset L^2(\mathbb{R}^d)$ the **Marzari-Vanderbilt localization functional** is

$$F_{MV}(w) := \sum_{a=1}^{m} \int_{\mathbb{R}^d} |x|^2 |w_a(x)|^2 dx - \sum_{a=1}^{m} \sum_{j=1}^{d} \left(\int_{\mathbb{R}^d} x_j |w_a(x)|^2 dx \right)^2 .$$

Definition A system of **maximally localized composite Wannier functions (MLWF)** is:
a **minimizer** $\{w_1, \ldots, w_m\}$ of the Marzari-Vanderbilt localization functional in the set $\mathcal{W}^m := (\mathcal{D}(H) \cap \mathcal{D}(X))^m$ under the **constraint** that $\{\varphi_1, \ldots, \varphi_m\}$, for $\varphi_a = \widetilde{\mathcal{U}} w_a$, is a **Bloch frame** .

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Since [Marzari-Vanderbilt 97] this approach has been extremely successful in computational physics, see the recent review

Marzari et al., *Maximally localized Wannier functions: theory and applications*, submitted to Rev. Mod. Physics, arXiv:1112.541.

There are has been convincing **numerical evidence that MLWF are exponentially localized**, *i.e.* there exist $\beta > 0$ such that

$$\int_{\mathbb{R}^d} \mathrm{e}^{2\beta|x|} \, |w_a(x)|^2 dx < +\infty \qquad a \in \{1, \ldots, m\}.$$

Beyond numerical results, no mathematical proof . . .

Natural mathematical problems

(MV_1) **(Existence)** prove that there exists a system of maximally localized composite Wannier functions;

(MV_2) **(Localization)** prove that any maximally localized composite Wannier function is exponentially localized

The MV functional in momentum space

Since the modified Bloch-Floquet transform is an isometry and it satisfies

$$(\tilde{\mathcal{U}} X_j\, g)(k, y) = \mathrm{i} \frac{\partial}{\partial k_j} (\tilde{\mathcal{U}}\, g)(k, y)$$

the **MV functional can be rewritten in terms of the Bloch frame** $\varphi = \{\varphi_1, \ldots, \varphi_m\}$ as

$$\tilde{F}_{MV}(\varphi) = \sum_{a=1}^{m} \sum_{j=1}^{d} \left\{ \int_{\mathbb{B}} dk \int_{\mathbb{T}_Y} \left| \frac{\partial \varphi_a}{\partial k_j}(k, y) \right|^2 dy - \left(\int_{\mathbb{B}} dk \int_{\mathbb{T}_Y} \overline{\varphi_a(k, y)}\, i \frac{\partial \varphi_a}{\partial k_j}(k, y)\, dy \right)^2 \right\} .$$

The **minimization space** $\mathcal{W} = \mathcal{D}(H) \cap \mathcal{D}(X)$ is mapped by the Bloch-Floquet transform into

$$\mathcal{H}_\tau \cap L^2_{\mathrm{loc}}(\mathbb{R}^d, W^{2,2}(\mathbb{T}_Y)) \cap W^{1,2}_{\mathrm{loc}}(\mathbb{R}^d, L^2(\mathbb{T}_Y)) =: \widetilde{\mathcal{W}}.$$

The MV functional for the **unitary gauge**

It is convenient to use the **existence of a real-analytic Bloch frame** $\chi = \{\chi_1, \dots, \chi_m\}$ and rewrite the functional in terms of the **unknown change of gauge**, *i.e.*

$$\varphi_a(k, \cdot) = \sum_b \chi_b(k, \cdot)\, U_{b,a}(k) \qquad \text{with } U_{b,a}(k) = \langle \chi_b(k) \,|\, \varphi_a(k) \rangle_{\mathcal{H}_\mathrm{f}}$$

Here χ **is fixed**, and the **minimization variable** is the map

$$U \in W^{1,2}(\mathbb{T}^*_d, \mathcal{U}(\mathbb{C}^m)) \qquad \text{where } \mathbb{T}^*_d \equiv \mathbb{R}^d / \Gamma^*$$

The MV functional for the **unitary gauge**

For the given reference frame χ, the **localization functional** in terms of the gauge U reads

$$\begin{aligned}
\tilde{F}_{MV}(U;\chi) \;=\; & \sum_{j=1}^{d}\int_{\mathbb{T}_d^*}\left[\operatorname{tr}\left(\frac{\partial U^*}{\partial k_j}(k)\frac{\partial U}{\partial k_j}(k)\right) + m\sum_{a=1}^{m}\left\|\frac{\partial \chi_a(k,\cdot)}{\partial k_j}\right\|_{\mathcal{H}_f}^2\right] dk \;+ \\
& + \sum_{j=1}^{d}\int_{\mathbb{T}_d^*}\operatorname{tr}\left[\left(U(k)\frac{\partial U^*}{\partial k_j}(k) - \frac{\partial U}{\partial k_j}(k)U^*(k)\right)A_j(k)\right] dk \;+ \\
& + \sum_{a=1}^{m}\sum_{j=1}^{d}\left(\int_{\mathbb{T}_d^*}\left[U^*(k)\left(\frac{\partial U}{\partial k_j}(k) + A_j(k)U(k)\right)\right]_{aa} dk\right)^2 .
\end{aligned}$$

Here the matrix coefficients $A_j \in L^2(\mathbb{T}_d^*;\mathfrak{u}(m))$ are given by the formula

$$\left[A_j(k)\right]_{cb} = \left\langle \chi_c(k,\cdot)\,\middle|\,\frac{\partial \chi_b(k,\cdot)}{\partial k_j}\right\rangle_{\mathcal{H}_f} - \left\langle \frac{\partial \chi_c(k,\cdot)}{\partial k_j}\,\middle|\,\chi_b(k,\cdot)\right\rangle_{\mathcal{H}_f} .$$

The MV functional for the **unitary gauge**

For the given reference frame χ, the **localization functional** in terms of the gauge U reads

$$\begin{aligned} \tilde{F}_{MV}(U;\chi) = & \sum_{j=1}^{d} \int_{\mathbb{T}_d^*} \left[\operatorname{tr}\left(\frac{\partial U^*}{\partial k_j}(k) \frac{\partial U}{\partial k_j}(k) \right) + m \sum_{a=1}^{m} \left\| \frac{\partial \chi_a(k,\cdot)}{\partial k_j} \right\|_{\mathcal{H}_f}^2 \right] dk \; + \\ & + \sum_{j=1}^{d} \int_{\mathbb{T}_d^*} \operatorname{tr}\left[\left(U(k) \frac{\partial U^*}{\partial k_j}(k) - \frac{\partial U}{\partial k_j}(k) U^*(k) \right) A_j(k) \right] dk \; + \\ & + \sum_{a=1}^{m} \sum_{j=1}^{d} \left(\int_{\mathbb{T}_d^*} \left[U^*(k) \left(\frac{\partial U}{\partial k_j}(k) + A_j(k) U(k) \right) \right]_{aa} dk \right)^2 . \end{aligned}$$

Beautiful!!! The former functional is a **perturbation of the Dirichlet energy for maps $U : \mathbb{T}_d^* \to \mathcal{U}(\mathbb{C}^m)$!**

In other words, stationary points are **harmonic maps**.

In summary

$$\inf\left\{ F_{MV}(w) \ :\ \begin{array}{c} \{w_1,\ldots,w_m\}\subset\mathcal{W} \\ \widetilde{\mathcal{U}}\, w \text{ is a Bloch frame} \end{array} \right\} = \inf\left\{ \tilde{F}_{MV}(U;\chi) \ :\ U\in W^{1,2}(\mathbb{T}^*_d;\mathcal{U}(\mathbb{C}^m)) \right\}.$$

Therefore, **problem** (MV$_1$) is equivalent to show that the r.h.s. is attained.

Analogously, **problem** (MV$_2$) corresponds to show that **any minimizer of** $\tilde{F}_{MV}(\cdot;\chi)$ **is real-analytic**, provided that χ is also real-analytic.

Theorem. [Panati & Pisante 11]
Let σ_* be a family of m Bloch bands for the operator $-\Delta + V_\Gamma$ satisfying the gap condition, and let $\{P_*(k)\}_{k\in\mathbb{R}^d}$ be the corresponding family of spectral projectors.
Assume $d \leq 2$ and $m \geq 1$, or $d \geq 1$ and $m = 1$, or $d = 3$ and $1 \leq m \leq 15$.
Then:

- (MV$_1$) there exist composite Wannier functions $\{w_1, \ldots, w_m\} \subset \mathcal{W}$ which **minimize the localization functional** under the constraint that the corresponding quasi-Bloch functions are an orthonormal basis for Ran $P_*(k)$ for each $k \in \mathbb{B}$.
- (MV$_2$) for any system of maximally localized composite Wannier function $w = \{w_1, \ldots, w_m\}$ there exists $\beta > 0$ such that $e^{\beta|x|}w_a$ is in $L^2(\mathbb{R}^d)$ for every $a \in \{1, \ldots, m\}$, *i.e.* **the composite Wannier function w_a is exponentially localized.**

Conjecturally, we expect that the **parameter β appearing in the latter claim does not depend on the minimizer** w, and that the claim holds true for any $\beta < \alpha$, where α is the **width of the analyticity strip** for $k \mapsto P_*(k)$.

We also expect that the result holds true **for any $m \in \mathbb{N}$ even for $d = 3$.**

Snapshots from the proof

- The **existence of a minimizer is standard**, it follows essentially from the direct method of calculus of variations
- We prove the analyticity of the minimizers of $\tilde{F}_{\mathrm{MV}}$ by adapting ideas and methods from the **regularity theory for harmonic maps** **[Chan Wang & Yang][Lin & Wang]**
- The crucial step is to prove that any minimizer of $\tilde{F}_{\mathrm{MV}}$ is **continuous**.
- In the 2-dimensional case, this fact is a consequence of the **hidden structure of the nonlinear terms in the Euler Lagrange equation** for the $\tilde{F}_{\mathrm{MV}}$ functional.
- In the 3-dimensional case, the continuity follows instead from the deeper fact that **minimizers at smaller and smaller scales look like minimizing harmonic maps from** $\mathbb{T}_d^*$ to $\mathcal{U}(\mathbb{C}^m)$. We are able to prove that, for $m \leq 15$, the latter are actually real-analytic, by showing constancy of the tangent maps as in **[Schoen & Uhlenbeck 84]**.
  As a consequence, we obtain the continuity of the minimizers of $\tilde{F}_{\mathrm{MV}}$.

The Euler-Lagrange equations

Let $\varphi \in C^\infty(\mathbb{T}_d^*; M_m(\mathbb{C}))$ and for $\varepsilon \neq 0$ fixed let

$U(k) + \varepsilon\varphi(k)$ be **a free variation of U in the direction φ**.

In a sufficiently small tubular neighborhood $\mathcal{O}$ of $\mathcal{U}(m)$ in $M_m(\mathbb{C})$ there is a well defined **nearest point projection map** $\Pi : \mathcal{O} \longrightarrow \mathcal{U}(m)$, so the **projected variations** are

$$U_\varepsilon(k) := \Pi(U(k)+\varepsilon\varphi(k)) = U(k)\left(\mathbb{I} + \varepsilon\frac{1}{2}\left[U^{-1}(k)\varphi(k) - (U^{-1}(k)\varphi(k))^*\right]\right)+o(\varepsilon)\,.$$

Lemma. A map $U \in W^{1,2}(\mathbb{T}_d^*;\mathcal{U}(m))$ satisfies $\frac{d}{d\varepsilon}\tilde{F}_{MV}(U_\varepsilon;\chi)|_{\varepsilon=0} = 0$ if and only if U is a weak solution of the **Euler-Lagrange equation**

$$-\Delta U + \sum_{j=1}^{d} \frac{\partial U}{\partial k_j}U^{-1}\frac{\partial U}{\partial k_j} + \sum_{j=1}^{d}\left[\frac{\partial U}{\partial k_j}U^{-1}A_jU - \frac{\partial A_j}{\partial k_j}U - A_j\frac{\partial U}{\partial k_j}\right] +$$

$$+\sum_{j=1}^{d}\left[-\left(\frac{\partial U}{\partial k_j} + A_jU\right)G^j + UG^jU^{-1}\left(\frac{\partial U}{\partial k_j} + A_jU\right)\right] = 0\,.$$

Here the constant (purely imaginary) diagonal matrices $\{G^j\} \subset M_m(\mathbb{C})$ are defined as

$$G^j = \operatorname{diag} \int_{\mathbb{T}_d^*} U^*(k) \left[\frac{\partial U}{\partial k_j}(k) + A_j(k) U(k) \right] dk.$$

Continuity in the 2-dimensional case

Crucial lemma. [P & Pisante] borrowing ideas from [Lin & Wang]

Let $d \geq 2$, $m \geq 2$ and let $U \in W^{1,2}(\mathbb{T}^*_d; \mathcal{U}(m))$.

Assume $\tilde{B}^j \in L^2(\mathbb{T}^*_d; \mathfrak{u}(m))$ for $j \in \{1, \dots, d\}$ and $\operatorname{div} \tilde{B} = 0$ in $\mathcal{D}'(\mathbb{T}^*_d)$.

If U **is a weak solution to**

$$\Delta U = \sum_{j=1}^{d} \frac{\partial U}{\partial k_j} \tilde{B}^j + \tilde{f} \qquad \text{and } U^{-1}\tilde{f} \in L^p(\mathbb{T}^*_d; \mathfrak{u}(m))$$

for some $p > 1$, **then** $U \in W^{2,1}(\mathbb{T}^*_d; \mathcal{U}(m))$.

The Euler-Lagrange equations can be recast in the form above. For $d = 2$ one has **continuity by Sobolev embedding**.

Continuity in the 3-dimensional case

Let $\Omega' \subset \mathbb{R}^d$ an open set, $d \geq 3$, and let $U \in W^{1,2}_{\mathrm{loc}}(\Omega'; \mathcal{U}(m))$, $\; m \geq 2$.

Define the **Dirichlet energy**

$$E(U;\Omega) = \int_\Omega \frac{1}{2} \sum_{j=1}^{d} \mathrm{tr}\left(\frac{\partial U^*}{\partial k_j} \frac{\partial U}{\partial k_j} \right) dk \,, \qquad \Omega \subset\subset \Omega'.$$

The condition of stationarity for E easily implies that **U is a weakly harmonic map**, *i. e.* U is a weak solution of

$$-\Delta U + \sum_{j=1}^{d} \frac{\partial U}{\partial k_j} U^{-1} \frac{\partial U}{\partial k_j} = 0 \,.$$

We aim to prove that, when $d = 3$ and $m \geq 2$ **any local minimizer $U \in W^{1,2}_{\mathrm{loc}}(\mathbb{R}^3; \mathcal{U}(m))$ which is degree-zero homogeneous,** *i. e.*

$$U(k) = \omega\left(\frac{k}{|k|} \right) \qquad \text{for some } \omega \in C^\infty(S^2; \mathcal{U}(m))$$

is constant.

Proposition [P & Pisante]

Let $m \geq 2$ and $\omega \in C^\infty(S^2; \mathcal{U}(m))$ a harmonic map. If $U(k) = \omega\left(\frac{k}{|k|}\right)$ is a **local minimizer of the Dirichlet energy** then the homogeneous energy satisfies

$$\mathcal{E}(\omega) \leq \frac{\pi}{2} m.$$

Here the homogeneous energy is the **Dirichlet energy for maps** $S^2 \to \mathcal{U}(m)$

$$\mathcal{E}(\omega) = \int_{S^2} \frac{1}{2} \left|\omega^{-1} d\omega\right|^2 dVol\,.$$

Proposition [Valli 88]. The energy $\mathcal{E}(\omega)$ of any harmonic map $\omega : S^2 \longrightarrow \mathcal{U}(m)$ is **an integer multiple of** 8π.

Obvious corollary. If $m \leq 15$ then $\mathcal{E}(\omega) = 0$, so ω is constant.

Details, proofs & applications in the preprint:
Bloch bundles, Marzari-Vanderbilt functional and maximally localized Wannier functions,
`arXiv:1112.6197`

Thank you
for you attention!!