BLOCH BUNDLES, MARZARI-VANDERBILT FUNCTIONAL AND MAXIMALLY LOCALIZED WANNIER FUNCTIONS

GIANLUCA PANATI AND ADRIANO PISANTE

Abstract. We consider a periodic Schrödinger operator and the composite Wannier functions corresponding to a relevant family of its Bloch bands, separated by a gap from the rest of the spectrum. We study the associated localization functional introduced in [MaVa] and we prove some results about the existence and exponential localization of its minimizers, in dimension $d \leq 3$. The proof exploits ideas and methods from the theory of harmonic maps between Riemannian manifolds.

Contents

1. Introduction

Many transport properties of electrons in crystalline solids are understood by the analysis of Schrödinger operators in the form

$$H = -\Delta + V_\Gamma(x) \qquad \text{acting in } L^2(\mathbb{R}^d) \tag{1.1}$$

where the function $V_\Gamma : \mathbb{R}^d \to \mathbb{R}$ is periodic with respect to a Bravais lattice $\Gamma \simeq \mathbb{Z}^d$. The function V_Γ represents (in Rydberg units) the electrostatic potential experienced by a test electron and generated by the ionic cores of the crystalline solid and, in a mean-field approximation, by the remaining electrons. We refer to [CaLeLi, CaDeLe] for the mathematical justification of such a model in the reduced Hartree-Fock approximation.

A crucial problem in solid state physics is the construction of an orthonormal basis, canonically associated to the operator H, consisting of functions which are exponentially localized in space. Indeed, such a basis allows to develop computational methods which scale linearly with the system size [Go], makes possible the description of the dynamics by *tight-binding* effective Hamiltonians [NaMa, HS], and plays a prominent role in the modern theories of macroscopic polarization [KSV, Re] and of orbital magnetization in crystalline solids [TCVR].

A convenient basis has been proposed by Wannier [Wa], and *Wannier functions* (see Definition 1) are nowadays a fundamental tool in solid state physics. The problem of proving the existence of exponentially localized Wannier functions was raised in 1959 by the Nobel Prize winner W. Kohn [Ko], who solved it in dimension $d = 1$ in the case of a single isolated Bloch band for a centrosymmetric potential. The latter condition has been later removed by J. des Cloizeaux [Cl2]. In higher dimension, the problem has been solved, always in the case of a single isolated Bloch band, by J. des Cloizeaux [Cl1, Cl2] for centrosymmetric potentials and finally by G. Nenciu under general hypotheses [Ne1], see also [HS] for a different proof and the review paper [Ne2]. As for dimension $d = 1$, an alternative approach based on the band position operator has been developed, yielding exponential localization of Wannier functions even for non periodic Schrödinger operators, see [NN, CNN] and references therein.

However, in dimension $d > 1$ the Bloch bands of crystalline solids are not, in general, isolated. Thus the interesting problem, in view of real applications, concerns the case of *multiband systems*, and in this context the more general notion of *composite Wannier functions* is relevant [Bl, Cl1]. The existence of exponentially localized composite Wannier functions has been proved in [Ne2] in dimension $d = 1$. As for $d > 1$, this problem remained unsolved until recently [Pa, BPCM], when an existence result was obtained by geometric methods.

To circumvent such conceptual difficulty, and in view of the application to numerical simulations, the solid-state physics community preferred to introduce the alternative notion of *maximally localized Wannier functions* [MaVa]. The latter are defined as the minimizers of a suitable localization functional, known as the Marzari-Vanderbilt (MV) functional. In [MaVa] it is also conjectured that the minimizers, whenever they exist, are exponentially localized. While such an approach provided excellent results from the numerical viewpoint, being nowadays an every-day tool in computational physics [MYSV, MSV], a mathematical analysis of the MV functional is still missing. Our goal is to fill this gap.

In this paper, we prove preliminarily that minimizers of the MV functional do exist for $d \leq 3$ in a suitable function space. More relevantly, we prove that the minimizers of the MV functional are exponentially localized. More precisely, let $m \geq 1$ be the number of Bloch bands corresponding to the composite Wannier functions; then the result is proved in three cases: if $m = 1$ for any $d \geq 1$, if $1 \leq d \leq 2$ for any $m \geq 1$, and if $d = 3$ under the constraint $2 \leq m \leq 3$ (Theorem 6.1). The proofs are dimension-dependent. In the first two cases, exponential localization holds true for any stationary point of the MV functional, *i.e.* for any solution of the corresponding Euler Lagrange equations, while in the three dimensional case the minimality property is crucial. In view of that, when $d = 3$ the constraint on m arises from the methods we exploit in the proof; we believe that it is purely technical, since we do not see any physical reason which prevents the result from being true for any $m \geq 1$. So far, even if one is merely interested in almost-exponential localization, *i.e.* to prove that the maximally localized composite Wannier functions decrease faster than the inverse of any polynomial, the constraint on m is needed in our approach.

The existence of a basis of Wannier functions which are exponentially localized in space is also relevant for the periodic Pauli and Dirac operators. The $\mathbb{Z}^d$-symmetry of the latter operators allows a direct integral decomposition analogous to the Bloch-Floquet transform, yielding a structure very similar to the one appearing for periodic Schrödinger operators. With few modifications, our methods can also be used to discuss the corresponding minimization problem in this context.

Mathematically, the MV functional can be rewritten, after Bloch-Floquet transform and by exploiting the time-reversal symmetry of the operator (1.1) (*i.e.* the fact that H commutes with the complex-conjugation operator), as a perturbation $\tilde{F}_{\mathrm{MV}}$ of the Dirichlet energy for maps from $\mathbb{T}_d^*$ to $\mathcal{U}(m)$, see (A.1), where $\mathbb{T}_d^* \simeq \mathbb{R}^d/(2\pi\mathbb{Z})^d$ is a d-dimensional flat torus and $\mathcal{U}(m) \subset \mathrm{M}_m(\mathbb{C})$ is the unitary group. The exponential localization of a minimizer of the MV functional is related to the analyticity of the corresponding minimizer of $\tilde{F}_{\mathrm{MV}}$. The existence of a minimizer of the latter functional 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, see [CWY, LW1, Si] and references therein. The crucial step is to prove that any minimizer of $\tilde{F}_{\mathrm{MV}}$ is continuous. In the two 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 three 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 $\mathcal{U}(m)$. We are able to prove that, for $m \leq 3$, the latter are actually real-analytic (Theorem A.11), by showing constancy of the tangent maps as in the important paper [SU2]. As a consequence, we obtain the continuity of the minimizers of $\tilde{F}_{\mathrm{MV}}$ and, in turn, analytic regularity.

We hope that our result will contribute to a fruitful exchange of ideas, problems and methods between the solid-state physics and the mathematics community, in the study of Schrödinger operators and related physical phenomena.

Acknowledgments. We are grateful to Ch. Brouder, G. Dell'Antonio and S. Teufel for a careful reading of the manuscript and for useful comments. We are indebted to A. D'Andrea, D. Fiorenza, G. Mondello and P. Papi for stimulating discussions about the geometric and Lie-theoretic aspects of the problem.

2. Wannier functions and Bloch bundles

2.1. **Periodic Schrödinger operators and Bloch-Floquet transform.** In this section we recall, following [PST], that, in view of their invariance under Γ-translations, Schrödinger operators in the form (1.1) can be decomposed as a direct integral of simpler operators by the (modified) Bloch-Floquet transform. A comparison with the formalism of the classical Bloch-Floquet transform, appearing in most of the physics literature, is summarized in Remark 2.6.

The lattice Γ, corresponding to the Bravais lattice in physics, is described as

$$\Gamma = \left\{ \gamma \in \mathbb{R}^d : \gamma = \textstyle\sum_{j=1}^d n_j \, \gamma_j \ \text{ for some } n_j \in \mathbb{Z} \right\},$$

where $\{\gamma_1, \dots, \gamma_d\}$ are fixed linearly independent vectors in $\mathbb{R}^d$. The dual lattice, with respect to the ordinary inner product, is $\Gamma^* := \left\{ k \in \mathbb{R}^d : \ k \cdot \gamma \in 2\pi\mathbb{Z} \text{ for all } \gamma \in \Gamma \right\}$. To fix the notation, we denote by Y the centered fundamental domain of Γ, namely

$$Y = \left\{ x \in \mathbb{R}^d : x = \textstyle\sum_{j=1}^d \alpha_j \, \gamma_j \ \text{ for } \alpha_j \in [-\tfrac{1}{2}, \tfrac{1}{2}] \right\}.$$

Analogously, we define the centered fundamental domain Y^* of Γ^* by setting

$$Y^* = \left\{ k \in \mathbb{R}^d : k = \textstyle\sum_{j=1}^d k'_j \, \gamma_j^* \ \text{ for } k'_j \in [-\tfrac{1}{2}, \tfrac{1}{2}] \right\},$$

where $\{\gamma_j^*\}$ is the dual basis to $\{\gamma_j\}$, *i.e.* $\gamma_j^* \cdot \gamma_i = 2\pi\delta_{j,i}$. When the opposite faces of Y^* are identified, one obtains the torus $\mathbb{T}_d^* := \mathbb{R}^d / \Gamma^*$, equipped with the flat Riemannian metric induced by $\mathbb{R}^d$.

For $\psi \in \mathcal{S}(\mathbb{R}^d)$, one defines the modified Bloch-Floquet transform as

$$(\tilde{\mathcal{U}}_{\mathrm{BF}} \psi)(k, y) := \frac{1}{|Y^*|^{\frac{1}{2}}} \sum_{\gamma \in \Gamma} \mathrm{e}^{-\mathrm{i}k \cdot (y + \gamma)} \, \psi(y + \gamma), \qquad y \in \mathbb{R}^d, \ k \in \mathbb{R}^d. \tag{2.1}$$

One immediately reads the periodicity properties

$$\begin{aligned} \big(\tilde{\mathcal{U}}_{\mathrm{BF}} \psi\big)(k, y + \gamma) &= \big(\tilde{\mathcal{U}}_{\mathrm{BF}} \psi\big)(k, y) && \text{for all } \gamma \in \Gamma\,, \\ \big(\tilde{\mathcal{U}}_{\mathrm{BF}} \psi\big)(k + \lambda, y) &= \mathrm{e}^{-\mathrm{i}\lambda \cdot y} \, \big(\tilde{\mathcal{U}}_{\mathrm{BF}} \psi\big)(k, y) && \text{for all } \lambda \in \Gamma^*\,. \end{aligned} \tag{2.2}$$

For any fixed $k \in \mathbb{R}^d$, $\big(\tilde{\mathcal{U}}_{\mathrm{BF}} \psi\big)(k, \cdot)$ is a Γ-periodic function and can thus be regarded as an element of $\mathcal{H}_{\mathrm{f}} := L^2(\mathbb{T}^d)$, $\mathbb{T}^d$ being the flat torus $\mathbb{R}^d / \Gamma$. On the other hand, the second equation in (2.2) can be read as a pseudoperiodicity property, involving a unitary representation of the group Γ^*, given by

$$\tau : \Gamma^* \to \mathcal{U}(\mathcal{H}_{\mathrm{f}})\,, \quad \lambda \mapsto \tau(\lambda)\,, \quad \big(\tau(\lambda)\varphi\big)(y) = \mathrm{e}^{\mathrm{i}\lambda \cdot y} \varphi(y). \tag{2.3}$$

Following [PST], it is convenient to introduce the Hilbert space

$$\mathcal{H}_\tau := \left\{ \varphi \in L^2_{\mathrm{loc}}(\mathbb{R}^d, \mathcal{H}_{\mathrm{f}}) : \ \varphi(k - \lambda) = \tau(\lambda)\, \varphi(k) \ \ \forall \lambda \in \Gamma^*, \ \text{for a.e. } k \in \mathbb{R}^d \right\}, \tag{2.4}$$

equipped with the inner product

$$\langle \varphi, \, \psi \rangle_{\mathcal{H}_\tau} = \int_{Y^*} dk \, \langle \varphi(k), \, \psi(k) \rangle_{\mathcal{H}_{\mathrm{f}}}\,.$$

Obviously, there is a natural isomorphism between $\mathcal{H}_\tau$ and $L^2(Y^*, \mathcal{H}_{\rm f})$ given by restriction from $\mathbb{R}^d$ to Y^*. The map defined by (2.1) extends to a unitary operator

$$\tilde{\mathcal{U}}_{\rm BF} : L^2(\mathbb{R}^d) \longrightarrow \mathcal{H}_\tau \simeq \int_{Y^*}^{\oplus} \mathcal{H}_{\rm f}\, dk,$$

with inverse given by

$$\left(\tilde{\mathcal{U}}_{\rm BF}^{-1}\varphi\right)(x) = \frac{1}{|Y^*|^{\frac{1}{2}}} \int_{Y^*} dk\ \mathrm{e}^{\mathrm{i}k\cdot x}\varphi(k,[x]),$$

where $[\,\cdot\,]$ refers to the a.e. unique decomposition $x = \gamma_x + [x]$, with $\gamma_x \in \Gamma$ and $[x] \in Y$. Finally, from the definition (2.1) one easily checks that

$$\begin{aligned} &\psi \in W^{m,2}(\mathbb{R}^d),\ m \in \mathbb{N} \iff \tilde{\mathcal{U}}_{\rm BF}\,\psi \in L^2(Y^*, W^{m,2}(\mathbb{T}^d)), \\ &\langle x\rangle^m\,\psi \in L^2(\mathbb{R}^d),\ m \in \mathbb{N} \iff \tilde{\mathcal{U}}_{\rm BF}\,\psi \in \mathcal{H}_\tau \cap W^{m,2}_{\rm loc}(\mathbb{R}^d, L^2(\mathbb{T}^d)), \end{aligned} \tag{2.5}$$

where, as usual, $\langle x\rangle = (1+|x^2|)^{1/2}$.

The advantage of this construction is that the transformed Hamiltonian is a fibered operator over Y^*. To assure that $H = -\Delta + V_\Gamma$ is self-adjoint in $L^2(\mathbb{R}^d)$ on the domain $W^{2,2}(\mathbb{R}^d)$, we make the following Kato-type assumption on the Γ-periodic potential [RS, Theorem XIII.96]:

$$V_\Gamma \in L^2_{\rm loc}(\mathbb{R}^d) \text{ for } d \leq 3, \qquad V_\Gamma \in L^p_{\rm loc}(\mathbb{R}^d) \text{ with } p > d/2 \text{ for } d \geq 4. \tag{2.6}$$

One checks that

$$\tilde{\mathcal{U}}_{\rm BF}\, H\, \tilde{\mathcal{U}}_{\rm BF}^{-1} = \int_{Y^*}^{\oplus} dk\, H(k)$$

with fiber operator

$$H(k) = \big(-\mathrm{i}\nabla_y + k\big)^2 + V_\Gamma(y)\,, \qquad k \in \mathbb{R}^d, \tag{2.7}$$

acting on the k-independent domain $\mathcal{D}_0 = W^{2,2}(\mathbb{T}^d) \subset L^2(\mathbb{T}^d)$. Each fiber operator $H(k)$ is self-adjoint, has compact resolvent and thus pure point spectrum accumulating at infinity. The eigenvalues are labeled increasingly, *i.e.* $E_0(k) \leq E_1(k) \leq E_2(k) \leq \ldots$, and repeated according to their multiplicity. Since the fiber Hamiltonians are τ-covariant, see [PST], in the sense that

$$H(k+\lambda) = \tau(\lambda)^{-1}\, H(k)\, \tau(\lambda), \qquad \forall \lambda \in \Gamma^*, \tag{2.8}$$

the eigenvalues are Γ^*-periodic, *i.e.* $E_n(k+\lambda) = E_n(k)$ for all $\lambda \in \Gamma^*$.

We denote by $\sigma_*(k)$ the set $\{E_i(k) : n \leq i \leq n+m-1\}$, $k \in Y^*$, corresponding to a physically relevant family of m Bloch bands, and we assume the following *gap condition*:

$$\inf_{k \in \mathbb{T}^*_d} \operatorname{dist}\big(\sigma_*(k), \sigma(H(k)) \setminus \sigma_*(k)\big) > 0. \tag{2.9}$$

The following result borrows ideas in [Cl1, Cl2] and [Ne2, Theorem 3.3], where however a different definition of the Bloch-Floquet transform is used.

Proposition 2.1. *Let $P_*(k) \in \mathcal{B}(\mathcal{H}_{\rm f})$ be the spectral projector of $H(k)$ corresponding to the set $\sigma_*(k) \subset \mathbb{R}$. Assume that σ_* satisfies (2.9). Then the family $\{P_*(k)\}_{k\in\mathbb{R}^d}$ has the following properties:*

(P_1) *the map $k \mapsto P_*(k)$ is smooth from $\mathbb{R}^d$ to $\mathcal{B}(\mathcal{H}_{\rm f})$ (equipped with the operator norm);*

($\tilde{\mathrm{P}}_1$) *the map* $k \mapsto P_*(k)$ *extends to a* $\mathcal{B}(\mathcal{H}_{\mathrm{f}})$*-valued analytic function on the domain*

$$\Omega_\alpha = \Big\{ \kappa \in \mathbb{C}^d : \ |\mathrm{Im}(\kappa_j)| < \alpha \quad \forall j \in \{1, \dots, d\} \Big\} \tag{2.10}$$

for some $\alpha > 0$*;*

(P_2) *the map* $k \mapsto P_*(k)$ *is* τ*-covariant, i.e.*

$$P_*(k + \lambda) = \tau(\lambda)^{-1} \, P_*(k) \, \tau(\lambda) \qquad \forall k \in \mathbb{R}^d, \quad \forall \lambda \in \Gamma^*;$$

($\tilde{\mathrm{P}}_2$) *the map* $\kappa \mapsto P_*(\kappa)$ *is* τ*-covariant, i.e.*

$$P_*(\kappa + \lambda) = \tau(\lambda)^{-1} \, P_*(\kappa) \, \tau(\lambda) \qquad \forall \kappa \in \Omega_\alpha, \quad \forall \lambda \in \Gamma^*;$$

(P_3) *there exists an antiunitary operator* [(1)] C *acting on* $\mathcal{H}_{\mathrm{f}}$ *such that*

$$P_*(-k) = C \, P_*(k) \, C^{-1} \qquad \text{and} \qquad C^2 = 1.$$

While properties (P_1) and (P_2) are a consequence of the fact that the operator H commutes with the lattice translations, jointly with the gap condition (2.9), property (P_3) follows from the fact that the operator (1.1) is real, and corresponds to the time-reversal symmetry of the physical system. Notice that property (P_3) generically does not hold true for periodic *magnetic* Schrödinger operators.

Proof. One uses (2.7) to define $H(\kappa)$ for every $\kappa \in \mathbb{C}^d$. Since for any $\kappa_0 \in \mathbb{C}^d$ one has

$$H(\kappa) = H(\kappa_0) + 2(\kappa - \kappa_0) \cdot (-i\nabla_y) + (\kappa^2 - \kappa_0^2)\mathbf{1}$$

and $(-i\nabla_y)$ is $H(\kappa_0)$-bounded, the family $\{H(\kappa)\}_{\kappa \in \mathbb{C}^d}$ is an entire analytic family of type (A) [RS, Chapter XII]. Hence $\{H(\kappa)\}_{\kappa \in \mathbb{C}^d}$ is an entire analytic family in the sense of Kato [RS, Theorem XII.9]. As a consequence, the set

$$R = \Big\{ (\kappa, \lambda) \in \mathbb{C}^d \times \mathbb{C} : \ \lambda \in \rho(H(\kappa)) \Big\}$$

is an open set, and $(\kappa, \lambda) \mapsto (H(\kappa) - \lambda\mathbf{1})^{-1}$ is an analytic function on R. Since R is open and (2.9) holds, for every every $k_0 \in \mathbb{R}^d$ there exist a positively oriented circle $\Lambda(k_0) \subset \mathbb{C}$ and a neighborhood $N_{k_0} \subset \mathbb{C}^d$ of k_0, such that $\Lambda(k_0)$ separates $\sigma_*(\kappa)$ from the rest of the spectrum and $\Lambda(k_0) \subset \rho(H(\kappa))$ for every $\kappa \in N_{k_0}$. Then the Riesz's formula

$$P_*(\kappa) = \frac{i}{2\pi} \oint_{\Lambda(k_0)} (H(\kappa) - z\mathbf{1})^{-1} dz \tag{2.11}$$

defines a map $\kappa \mapsto P_*(\kappa)$ which is analytic in N_{k_0}. For $\kappa = k \in N_{k_0} \cap \mathbb{R}^d$, it agrees with the spectral projection $P_*(k)$, so (P_1) holds true.

Since σ_* is Γ^*-periodic, the circle in (2.11) can be chosen so that $\Lambda(k_0) = \Lambda(k_0 + \lambda)$ for every $\lambda \in \Gamma^*$. Thus, property (P_2) follows from (2.8) and (2.11).

Formula (2.11) yields a $\mathcal{B}(\mathcal{H}_{\mathrm{f}})$-valued analytic function on $\cup_{k_0} N_{k_0} \supset \mathbb{R}^d$. In view of ($\mathrm{P}_2$) and the unique continuation principle, one may assume $N_{k_0 + \lambda} = N_{k_0}$ for every $\lambda \in \Gamma^*$, so by the compactness of Y^* there exist $\alpha > 0$ such that $\cup_{k_0} N_{k_0} \supset \Omega_\alpha$, *i.e.* ($\tilde{\mathrm{P}}_1$) holds true. Moreover, in view of (P_2) and the unique continuation principle, one gets ($\tilde{\mathrm{P}}_2$).

[(1)] By *antiunitary* operator we mean a surjective antilinear operator $C : \mathcal{H} \to \mathcal{H}$, such that $\langle C\varphi, C\psi \rangle_{\mathcal{H}} = \langle \psi, \varphi \rangle_{\mathcal{H}}$ for any $\varphi, \psi \in \mathcal{H}$.

Property (P_3) corresponds to time-reversal symmetry. This symmetry is realized in $L^2(\mathbb{R}^d)$ by the complex conjugation operator, acting as $(T\psi)(x) = \overline{\psi(x)}$ for $\psi \in L^2(\mathbb{R}^d)$. One directly checks that $\tilde{T} = \tilde{\mathcal{U}}_{\mathrm{BF}}\, T\, \tilde{\mathcal{U}}_{\mathrm{BF}}^{-1}$ acts on $\mathcal{H}_\tau \simeq L^2(Y^*, \mathcal{H}_{\mathrm{f}})$ as

$$(\tilde{T}\varphi)(k) = C\,\varphi(-k), \qquad\qquad \varphi \in L^2(Y^*, \mathcal{H}_{\mathrm{f}}),$$

where C is the complex conjugation operator in $\mathcal{H}_{\mathrm{f}}$. From the fact that H commutes with T, taking into account (2.9), property (P_3) follows, see [Pa] for details. □

2.2. **The Wannier functions and their localization properties.**

Case I. Simple Bloch band. We initially consider the case of a single isolated Bloch band, namely $\sigma_*(k) = \{E_n(k)\}$ and (2.9) is satisfied, such that $E_n(k)$ is an eigenvalue of multiplicity one for every k. This case corresponds to the "simple direct isolated band " in [Ne2].

A (normalized) **Bloch function** corresponding to the n-th Bloch band is, by definition, any $\varphi \in \mathcal{H}_\tau$ satisfying

$$\varphi(k,\cdot) \in \mathcal{D}_0 \qquad H(k)\varphi(k,\cdot) = E_n(k)\varphi(k,\cdot) \quad \text{and} \quad \|\varphi(k,\cdot)\|_{\mathcal{H}_{\mathrm{f}}} = 1 \qquad \forall k \in Y^*. \tag{2.12}$$

Clearly, if φ is a Bloch function then $\tilde{\varphi}$, defined by $\tilde{\varphi}(k,y) = \mathrm{e}^{\mathrm{i}\vartheta(k)}\varphi(k,y)$ for any function $\vartheta : \mathbb{T}^*_d \to \mathbb{R}$, is also a Bloch function. The latter invariance is often called *Bloch gauge invariance*. Notice that (2.12) is equivalent to

$$P_*(k)\varphi(k,\cdot) = \varphi(k,\cdot) \quad \text{and} \quad \|\varphi(k,\cdot)\|_{\mathcal{H}_{\mathrm{f}}} = 1 \qquad \forall k \in Y^*, \tag{2.13}$$

where $P_*(k)$ is the rank-one projection on the eigenspace corresponding to the eigenvalue $E_n(k)$.

Definition 1. *The* ***Wannier function*** $w_n \in L^2(\mathbb{R}^d)$ *corresponding to a Bloch function* $\varphi_n \in \mathcal{H}_\tau$ *for the Bloch band* E_n *is the preimage of* φ_n *with respect to the Bloch-Floquet transform, namely*

$$w_n(x) := \left(\tilde{\mathcal{U}}_{\mathrm{BF}}^{-1}\varphi_n\right)(x) = \frac{1}{|Y^*|^{\frac{1}{2}}}\int_{Y^*} dk\ \mathrm{e}^{\mathrm{i}k\cdot x}\varphi_n(k,[x]).$$

The translated Wannier functions are

$$w_{n,\gamma}(x) := w_n(x-\gamma) = \frac{1}{|Y^*|^{\frac{1}{2}}}\int_{Y^*} dk\ \mathrm{e}^{-\mathrm{i}k\cdot\gamma}\ \mathrm{e}^{\mathrm{i}k\cdot x}\varphi_n(k,[x]), \qquad \gamma \in \Gamma.$$

Thus, in view of the orthogonality of the trigonometric polynomials and the fact that $\tilde{\mathcal{U}}_{\mathrm{BF}}$ is an isometry, the functions $\{w_{n,\gamma}\}_{\gamma\in\Gamma}$ are mutually orthogonal in $L^2(\mathbb{R}^d)$. Moreover, the family $\{w_{n,\gamma}\}_{\gamma\in\Gamma}$ is a complete orthonormal basis of $\tilde{\mathcal{U}}_{\mathrm{BF}}^{-1}\,(\operatorname{Ran} P_*)$, where $P_* = \int_{Y^*}^{\oplus} P_*(k)\,dk$ is the total projector corresponding to the Bloch band E_n. Notice that the previous definition and elementary properties do not rely on the gap condition (2.9).

The (weak) localization of w_n expressed by the fact that w_n is in $L^2(\mathbb{R}^d)$ is physically unsatisfactory, since it does not imply that the position operator and its powers have finite expectation value. Therefore, it is natural to search for conditions on φ_n which guarantee a stronger decay of w_n. In a nutshell, the localization properties of the Wannier function are determined by the regularity (continuity, smoothness, analyticity, ...) of the corresponding Bloch function. By a simple integration by parts, and an exact cancelation of the opposite boundary terms, one obtains the following lemma. Here X_j, for $j \in \{1, \dots, d\}$, denotes the the j^{th} component of the position operator, *i.e.* $(X_j\psi)(x) = x_j\,\psi(x)$ for ψ in a suitable dense subspace of $L^2(\mathbb{R}^d)$

Lemma 2.2. *Let $\varphi \in \mathcal{H}_\tau$, $\varphi \in C^1(\mathbb{R}^d, \mathcal{H}_{\mathrm{f}})$ and let $w = \tilde{\mathcal{U}}_{\mathrm{BF}}^{-1}\varphi$. Then $X_j w$ is in $L^2(\mathbb{R}^d)$ and*

$$\tilde{\mathcal{U}}_{\mathrm{BF}}(-\mathrm{i}X_j w) = \partial_{k_j}\varphi.$$

By iterating the previous lemma, and taking into account (2.5), one concludes that if $\varphi \in \mathcal{H}_\tau$ is in $C^\infty(\mathbb{R}^d, \mathcal{H}_{\mathrm{f}})$, then the corresponding Wannier function decreases faster than the inverse of any polynomial, *i.e.* $P(X_1, \dots, X_d)w$ is in $L^2(\mathbb{R}^d)$ for any polynomial P. As for the exponential localization, by mimicking the proof of the usual Paley-Wiener theorem one gets the following result, see also [Ku1] for a slightly different formulation.

Proposition 2.3. *Let Ω_β be defined by (2.10) and*

$$\mathcal{H}^{\mathbb{C}}_{\tau,\beta} = \left\{ \Phi \in L^2_{\mathrm{loc}}(\Omega_\beta, \mathcal{H}_{\mathrm{f}}) : \Phi(z - \lambda) = \tau(\lambda)\Phi(z) \text{ for all } \lambda \in \Gamma^*, z \in \Omega_\beta \right\}.$$

Let ϕ be the restriction to $\mathbb{R}^d$ of a function $\Phi \in \mathcal{H}^{\mathbb{C}}_{\tau,\beta}$ analytic in the strip Ω_β. Assume that

$$\int_{Y^*} \|\Phi(k + \mathrm{i}h)\|^2_{\mathcal{H}_{\mathrm{f}}}\, dk \le C \qquad \forall h \text{ with } |h_j| < \beta$$

with a constant C uniform in h. Then, the function $w := \tilde{\mathcal{U}}_{\mathrm{BF}}^{-1}\,\phi$ satisfies

$$\int_{\mathbb{R}^d} \mathrm{e}^{2\beta|x|}\,|w(x)|^2 dx < +\infty.$$

Sketch of the proof. Let $k + \mathrm{i}h$ be in Ω_β, and pose $\phi^h(k) := \Phi(k + \mathrm{i}h)$, so that $\phi_h \in \mathcal{H}_\tau$. By shifting the integration contour by the method of residues, and by the τ-equivariance of ϕ^h, one gets

$$w^h(x) := \left(\tilde{\mathcal{U}}_{\mathrm{BF}}^{-1}\phi^h\right)(x) = \int_{Y^*} dk\, \mathrm{e}^{\mathrm{i}k\cdot x}\,\Phi(k + \mathrm{i}h, [x]) = \mathrm{e}^{h\cdot x} w(x).$$

Then, by the unitarity of $\tilde{\mathcal{U}}_{\mathrm{BF}}$,

$$\|\mathrm{e}^{h\cdot x} w\|^2_{L^2(\mathbb{R}^d)} = \int_{Y^*} \|\Phi(k + \mathrm{i}h)\|^2_{\mathcal{H}_{\mathrm{f}}}\, dk \le C.$$

Since the latter constant does not depend on h for $|h_j| \le \beta$, one has $\|\mathrm{e}^{\beta|x|} w\|_{L^2(\mathbb{R}^d)} < +\infty$. □

Corollary 2.4. *Let ϕ be the restriction to $\mathbb{R}^d$ of a function $\Phi \in \mathcal{H}^{\mathbb{C}}_{\tau,\alpha}$ analytic in the strip Ω_α. Then, for every $\beta < \alpha$, the function $w := \tilde{\mathcal{U}}_{\mathrm{BF}}^{-1}\,\phi$ satisfies*

$$\int_{\mathbb{R}^d} \mathrm{e}^{2\beta|x|}\,|w(x)|^2 dx < +\infty. \tag{2.14}$$

A function $w \in L^2(\mathbb{R}^d)$ satisfying (2.14) for some $\beta > 0$ is said to be ***exponentially localized***, while a function $w \in L^2(\mathbb{R}^d)$ such that $P(X_1, \dots, X_d)w$ is in $L^2(\mathbb{R}^d)$ for any polynomial P is said ***almost-exponentially localized***.

In view of the previous proposition, the existence of an exponentially (resp. almost-exponentially) localized Wannier function for the Bloch band E_n is equivalent to the existence of an analytic (resp. smooth) Bloch function. Property $(\tilde{\mathrm{P}}_1)$ (resp. (P_1)) assures that there is a choice of the Bloch gauge such that the Bloch function is analytic (resp. smooth) around a given point. However, as several authors noticed [Cl1, Ne2], there might be a topological obstruction to obtaining a global analytic (resp. smooth) Bloch function, in view of the competition between the regularity and the τ-equivariance (remember that the Bloch function must be in $\mathcal{H}_\tau$ by definition). This topological obstruction will be encoded in the concept of Bloch bundle, which we will introduce in the next subsection. Preliminarily, we describe the more realistic case of the composite Bloch bands.

Case II. Composite Bloch bands. We consider now the generic case of a family σ_* of m Bloch bands satisfying (2.9). Since the eigenvalues in the family σ_* generically intersect each other, and the eigenprojectors of $H(k)$ corresponding to single eigenvalues are not smooth at the intersection point, generically it is not even possible to find a system of locally smooth Bloch functions spanning $\operatorname{Ran} P_*(k)$ at any k close to a given k_0. Thus, the notion of Bloch function is relaxed and replaced by the following one [Bl, Cl1].

Definition 2. *Let* $\{P_*(k)\}_{k\in\mathbb{R}^d} \subset \mathcal{B}(\mathcal{H}_{\mathrm{f}})$ *be a family of orthogonal projectors satisfying* (P_1) *and* (P_2)*, with* $\dim P_*(k) \equiv m < +\infty$*. A function* $\chi \in \mathcal{H}_\tau$ *is called a* ***quasi-Bloch function*** *(for the family* $\{P_*(k)\}$*) if*

$$P_*(k)\chi(k,\cdot) = \chi(k,\cdot) \quad \text{and} \quad \chi(k,\cdot) \neq 0 \qquad \forall k \in Y^*. \tag{2.15}$$

A ***Bloch frame*** *(for the family* $\{P_*(k)\}$*) is a set* $\{\chi_a\}_{a=1,\dots,m}$ *of quasi-Bloch functions such that* $\{\chi_1(k),\dots,\chi_m(k)\}$ *is an orthonormal basis of* $\operatorname{Ran} P_*(k)$ *at (almost-)every* $k \in Y^*$*.*

A Bloch frame is fixed only up to a k-dependent unitary matrix $U(k) \in \mathcal{U}(m)$, *i.e.* if $\{\chi_a\}_{a=1,\dots,m}$ is a Bloch frame then the functions $\widetilde{\chi}_a(k) = \sum_{b=1}^m \chi_b(k) U_{b,a}(k)$ also define a Bloch frame.

Definition 3. *The* ***composite Wannier functions*** *corresponding to a Bloch frame* $\{\chi_a\}_{a=1}^m$ *are the functions*

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

As in the case of a single Bloch band, the existence of a system of exponentially localized (resp. almost-exponentially localized) composite Wannier function is equivalent to the existence of an analytic (resp. smooth) Bloch frame. The topological obstruction to the existence of a regular (analytic, smooth or continuous) Bloch frame, already observed in [Cl1, Ne2] is described in the next subsection.

Remark 2.5 (**Regularity of composite Wannier functions**)**.** We emphasize that, for V_Γ satisfying (2.6), the composite Wannier functions are actually in $W^{2,2}(\mathbb{R}^d)$ and, in general, one cannot expect better regularity properties. For example, if V_Γ has a Coulomb singularity, the Wannier functions are not smooth, as it happens for the eigenfunctions of the hydrogen atom.

To study the regularity properties of w_a, one notices that the corresponding quasi-Bloch function $\psi_a(k)$ is in $W^{2,2}(\mathbb{T}^d)$ and $\|\psi_a(k)\|_{W^{2,2}(\mathbb{T}^d)} \leq C_m \|\psi_a(k)\|_{L^2(\mathbb{T}^d)}$. Indeed, one can check that the previous inequality is a consequence of the fact that V_Γ corresponds to a multiplication operator in $L^2(\mathbb{T}^d)$ which is Δ-bounded with relative bound zero, together with the fact that the union of the ranges of the functions $\{E_i \,:\, n \leq i \leq n+m-1\}$ is contained in a fixed compact set. As a consequence, in view of (2.5), one concludes that $w_a \in W^{2,2}(\mathbb{R}^d)$, namely w_a is in the domain of H.

Remark 2.6 (**Comparison with the physics literature**)**.** When comparing our definitions with the physics literature, one has to take into account that we are using a *modified* Bloch-Floquet transform, so that the fiber Hamiltonian (2.7) has a k-independent domain. This fact is convenient from the mathematical viewpoint. Alternatively, the classical Bloch-Floquet transform

$$(\mathcal{U}_{\mathrm{BF}}\psi)(k,y) := \frac{1}{|Y^*|^{\frac{1}{2}}} \sum_{\gamma\in\Gamma} \mathrm{e}^{-\mathrm{i}k\cdot\gamma}\, \psi(y+\gamma), \qquad k \in \mathbb{R}^d, \quad y \in \mathbb{R}^d, \tag{2.16}$$

yields a decomposition $\mathcal{U}_{\mathrm{BF}}\,(-\Delta + V_\Gamma)\,\mathcal{U}_{\mathrm{BF}}^{-1} = \int_{\mathbb{T}_d^*}^{\oplus} H_{\mathrm{cl}}(k)\,dk$ where $H_{\mathrm{cl}}(k) = -\Delta + V_\Gamma$ acts in

$$\mathcal{H}_k := \left\{ \psi \in L^2_{\mathrm{loc}}(\mathbb{R}^d) : \psi(y+\gamma) = \mathrm{e}^{\mathrm{i}k\cdot\gamma}\psi(y) \quad \forall\gamma\in\Gamma \quad \text{for a.e. } y \in \mathbb{R}^d \right\}$$

on the domain $\mathcal{D}_k := W^{2,2}_{\mathrm{loc}}(\mathbb{R}^d) \cap \mathcal{H}_k$. The unitary operator $\mathcal{J} = \mathcal{U}_{\mathrm{BF}}\,\tilde{\mathcal{U}}_{\mathrm{BF}}^{-1}$ acts as $(\mathcal{J}\varphi)\,(k,y) = \mathrm{e}^{\mathrm{i}k\cdot y}\varphi(k,y)$, is a fibered operator and its fiber, denoted by $J(k)$, maps unitarily the space $\mathcal{H}_{\mathrm{f}}$ into the space $\mathcal{H}_k$. Since $J(k)H_{\mathrm{cl}}(k)J(k)^{-1} = H(k)$, the operators $H(k)$ and $H_{\mathrm{cl}}(k)$ have the same spectrum $\{E_n(k)\}_{n\in\mathbb{N}}$.

In the physics literature, usually a Bloch function is defined as an eigenfunction $\psi_n(k,\cdot) \in \mathcal{D}_k$ of $H_{\mathrm{cl}}(k) = -\Delta + V_\Gamma$ for the eigenvalue $E_n(k)$. By the unitary equivalence above, the so-called *Bloch theorem*, one has that $\psi_n(k,y) = \mathrm{e}^{\mathrm{i}k\cdot y}\varphi_n(k,y)$, where $\varphi_n(k,\cdot)$ is Γ-periodic and $\varphi_n \in \mathcal{H}_\tau$. The latter is our Bloch function, as defined by (2.12). Consequently, in the physics literature the Wannier function is defined as $w_n = \mathcal{U}_{\mathrm{BF}}^{-1}\psi_n = \tilde{\mathcal{U}}_{\mathrm{BF}}^{-1}\varphi_n$, which coincides exactly with our definition.

2.3. **The Bloch bundle.**

To describe the geometric obstruction to the existence of a continuous, smooth or analytic Bloch frame it is convenient to introduce the concept of Bloch bundle, following [Pa]. In this subsection we assume as given a family of orthogonal projectors $\{P_*(k)\}_{k\in\mathbb{R}^d}$ satisfying properties (P_1), (P_2) and (P_3), or their complex counterparts. Notice that we could also abstract from the specific case of the operator (1.1) and consider such properties as convenient starting assumptions. Within this viewpoint, our approach can be applied to the periodic Pauli or Dirac operator, with obvious modifications.

Proposition 2.7. *To a family of orthogonal projectors* $\{P_*(k)\}_{k\in\mathbb{R}^d}$ *satisfying* (P_1) *and* (P_2) *is canonically associated a Hermitian smooth vector bundle* $\mathcal{E}_*$ *over* $\mathbb{T}_d^*$*, called the* Bloch bundle. *If* ($\tilde{\mathrm{P}}_1$) *and* ($\tilde{\mathrm{P}}_2$) *are also satisfied, then* $\mathcal{E}_*$ *is the restriction to* $\mathbb{T}_d^* = \mathbb{R}^d/\Gamma^*$ *of a holomorphic Hermitian vector bundle* $\tilde{\mathcal{E}}_*$ *over* Ω_α/Γ^*.

Proof. The idea of the construction is to firstly consider $\sqcup_{k\in\mathbb{R}^d} \operatorname{Ran} P_*(k)$ as a subbundle of the trivial bundle $\mathbb{R}^d \times \mathcal{H}_{\mathrm{f}}$ over $\mathbb{R}^d$. Then we use the τ-equivariance of the projectors to obtain a (quotient) vector bundle $\mathcal{E}_*$ over the quotient space $\mathbb{T}_d^* = \mathbb{R}^d/\Gamma^*$.

To construct $\mathcal{E}_*$, one firstly introduces on the set $\mathbb{R}^d \times \mathcal{H}_{\mathrm{f}}$ the equivalence relation $\sim_\tau$, where

$$(k,\varphi) \sim_\tau (k',\varphi') \qquad \Leftrightarrow \qquad (k',\varphi') = (k+\lambda\,,\,\tau(\lambda)^{-1}\varphi) \quad \text{for some } \lambda \in \Gamma^*.$$

The equivalence class with representative (k,φ) is denoted by $[k,\varphi]$. Then the total space $\mathcal{E}_*$ of the vector bundle is defined by

$$\mathcal{E}_* := \left\{ [k,\varphi] \in (\mathbb{R}^d \times \mathcal{H}_{\mathrm{f}})/\!\sim_\tau : \quad \varphi \in \operatorname{Ran} P_*(k) \right\}.$$

This definition does not depend on the representative in view of the covariance property (P_2). The projection to the base space $\pi : \mathcal{E}_* \to \mathbb{T}^*_d$ is $\pi[k,\varphi] = \mu(k)$, where μ is the projection modulo Γ^*. One checks that $\mathcal{E}_* \xrightarrow{\pi} \mathbb{T}^*_d$ is a smooth complex vector bundle with typical fiber $\mathbb{C}^m$. In particular, the local triviality follows from (P_1) and the use of the Kato-Nagy formula. Indeed, for any $k_0 \in \mathbb{R}^d$ there exists a neighborhood $O_{k_0} \subset \mathbb{R}^d$ of k_0 such that $\|P_*(k) - P_*(k_0)\| < 1$ for any $k \in O_{k_0}$. Then by setting (Kato-Nagy's formula [Ka, Sec. I.6.8])

$$W(k) := \left(1 - (P_*(k) - P_*(k_0))^2\right)^{-1/2} \left(P_*(k)P_*(k_0) + (1 - P_*(k))(1 - P_*(k_0))\right) \tag{2.17}$$

one gets a smooth map $W : O_{k_0} \to \mathcal{U}(\mathcal{H}_{\mathrm{f}})$ such that $W(k)\, P_*(k_0)\, W(k)^{-1} = P_*(k)$. If $\{\chi_a\}_{a=1,\dots,m}$ is any orthonormal basis spanning $\mathrm{Ran}P_*(k_0)$, then $\varphi_a(k) = W(k)\chi_a$ is a smooth local orthonormal frame for $\mathcal{E}_*$, yielding the local triviality of the fibration $\mathcal{E}_* \xrightarrow{\pi} \mathbb{T}^*_d$.

The vector bundle $\mathcal{E}_*$ carries a natural Hermitian structure. Indeed, if $v_1, v_2 \in \mathcal{E}_*$ are elements of the fiber over $\mu(k) \in \mathbb{T}^*_d$ then, up to a choice of the representatives, one has $v_1 = [k,\varphi_1]$ and $v_2 = [k,\varphi_2]$, and one poses $\langle v_1, v_2\rangle_{\mathcal{E}_*} := \langle \varphi_1, \varphi_2\rangle_{\mathcal{H}_{\mathrm{f}}}$.

As for the analytic case, one introduces an equivalence relation $\sim_\tau$ over $\Omega_\alpha \times \mathcal{H}_{\mathrm{f}}$ as above. Then the total space of $\tilde{\mathcal{E}}_*$ is defined by

$$\tilde{\mathcal{E}}_* = \{[\kappa,\varphi] \in (\Omega_\alpha \times \mathcal{H}_{\mathrm{f}})/{\sim_\tau} : \quad \varphi \in \mathrm{Ran}\, P_*(\kappa)\}$$

which is independent of the representative in view of ($\tilde{\mathrm{P}}_2$). Local triviality follows again from formula (2.17). Indeed, for every $\kappa_0 \in \Omega_\alpha$ there exists a neighborhood $N_{\kappa_0} \subset \Omega_\alpha$ such that $\|P_*(\kappa) - P_*(\kappa_0)\| < 1$ for every $\kappa \in N_{\kappa_0}$; then, formula (2.17) yields a holomorphic map $W : N_{\kappa_0} \to \mathcal{U}(\mathcal{H}_{\mathrm{f}})$ such that $W(\kappa)P_*(\kappa_0)W(\kappa)^{-1} = P_*(\kappa)$. Notice that, since $P_*(\kappa)^* = P_*(\overline{\kappa})$, the operator $W(\kappa)$ is not unitary when $\kappa \notin \mathbb{R}^d \cap N_{\kappa_0}$.

Since $\kappa \mapsto P_*(\kappa)$ extends $k \mapsto P_*(k)$ by ($\tilde{\mathrm{P}}_1$), and both the maps are τ-covariant, $\mathcal{E}_* \to \mathbb{T}^*_d$ is clearly a restriction of $\tilde{\mathcal{E}}_* \to \Omega_\alpha/\Gamma^*$. The Hermitian structure over the vector bundle $\tilde{\mathcal{E}}_*$ is defined as in the smooth case. □

The vector bundle $\mathcal{E}_*$ is equipped with a natural $\mathfrak{u}(m)$-connection (*Berry connection*), induced by the trivial connection on the trivial vector bundle $(\mathbb{R}^d \times \mathcal{H}_{\mathrm{f}})/{\sim_\tau} \to \mathbb{T}^*_d$. The triviality of the latter is a consequence of the fact that $\mathcal{U}(\mathcal{H}_{\mathrm{f}})$ is contractible whenever $\mathcal{H}_{\mathrm{f}}$ is infinite-dimensional [Kui].

The Bloch bundle encodes the geometrical obstruction to the existence of a global smooth (resp. analytic) Bloch frame. Indeed, the following result is implicit in [Pa].

Theorem 2.8. *Let $\{P_*(k)\}_{k\in\mathbb{R}^d} \subset \mathcal{B}(\mathcal{H}_{\mathrm{f}})$ be a family of orthogonal projectors satisfying properties* (P_1) *(resp.* ($\tilde{\mathrm{P}}_1$)*) and* (P_2) *(resp.* ($\tilde{\mathrm{P}}_2$)*), with $\dim P_*(k) \equiv m < +\infty$. Then the following statements are equivalent:*

- (A) ***existence of a regular Bloch frame:*** *there exists a Bloch frame $\{\chi_a\}_{a=1,\dots,m}$ such that each χ_a is in $C^\infty(\mathbb{R}^d, \mathcal{H}_{\mathrm{f}})$ (resp. each χ_a is the restriction to $\mathbb{R}^d$ of a function $\tilde{\chi}_a \in \mathcal{H}^{\mathbb{C}}_{\tau,\alpha}$ analytic on Ω_α);*
- (B) ***triviality of the Bloch bundle:*** *the vector bundle $\mathcal{E}_*$, associated to the family $\{P_*(k)\}_{k\in\mathbb{R}^d}$ according to Proposition 2.7, is trivial in the category of smooth Hermitian vector bundles over $\mathbb{T}^*_d$ (resp. the vector bundle $\tilde{\mathcal{E}}_*$ is trivial in the category of holomorphic Hermitian vector bundles over Ω_α/Γ^*).*

The Bloch bundle can be trivial for reasons unrelated to time-reversal symmetry, as in some phases of the Haldane model [Ha, Pr]. On the other hand, as a consequence of [Pa], under the assumption of time-reversal symmetry the Bloch bundle is always trivial in low dimension, as stated in the following result.

Theorem 2.9. *Let $\{P_*(k)\}_{k\in\mathbb{R}^d} \subset \mathcal{B}(\mathcal{H}_{\mathrm{f}})$ be a family of orthogonal projectors satisfying properties* $(\tilde{\mathrm{P}}_1)$, $(\tilde{\mathrm{P}}_2)$ *and* (P_3). *Assume $d \leq 3$ and $m \geq 1$, or $d \geq 1$ and $m = 1$. Then there exists a Bloch frame $\{\chi_a\}_{a=1,\dots,m}$ such that each χ_a is real-analytic, i.e. $\chi_a \in C^\omega(\mathbb{R}^d, \mathcal{H}_{\mathrm{f}}) \cap \mathcal{H}_\tau$.*

Sketch of the proof. Since the family $\{P_*(k)\}_{k\in\mathbb{R}^d}$ satisfies properties (P_1), (P_2) and (P_3), in view of [Pa, Theorem 1] there exists a smooth Bloch frame $\chi = \{\chi_1, \dots, \chi_m\} \subset \mathcal{H}_\tau \cap C^\infty(\mathbb{R}^d, \mathcal{H}_{\mathrm{f}})$, *i.e.* the Bloch bundle is trivial as a smooth Hermitian vector bundle. Moreover, since $(\tilde{\mathrm{P}}_1)$ is also satisfied, $\{P_*(k)\}_{k\in\mathbb{R}^d}$ admits a holomorphic extension to Ω_α, see (2.10). Theorem 2 in [Pa] implies the existence of a family of holomorphic functions $\chi_a^{\mathbb{C}} : \Omega_\alpha \to \mathcal{H}_{\mathrm{f}}$, $\chi_a \in \mathcal{H}^{\mathbb{C}}_{\tau,\alpha}$, such that $\left\{\chi_1^{\mathbb{C}}(\kappa), \dots, \chi_m^{\mathbb{C}}(\kappa)\right\}$ is a (possibly non-orthonormal) basis of $\operatorname{Ran} P_*(\kappa)$ for every $\kappa \in \Omega_\alpha$. By restriction from Ω_α to $\mathbb{R}^d$, and by a Gram-Schmidt orthonormalization procedure, one gets a real-analytic Bloch frame $\{\chi_1, \dots, \chi_m\} \subset C^\omega(\mathbb{R}^d, \mathcal{H}_{\mathrm{f}}) \cap \mathcal{H}_\tau$. □

3. The Marzari-Vanderbilt localization functional

The long-lasting uncertainty about the existence of exponentially localized composite Wannier functions in three dimensions, settled only recently [BPCM, Pa], and the need of an approach suitable for numerical simulations, lead the solid state physics community to explore new paths. In an important paper [MaVa], Marzari and Vanderbilt introduced the following concept.

For a single-band normalized Wannier function $w \in L^2(\mathbb{R}^d)$, one defines the localization functional by

$$F_{MV}(w) = \sum_{j=1}^{d} \operatorname{Var}\left(X_j; |w(x)|^2 dx\right) = \int_{\mathbb{R}^d} |x|^2 |w(x)|^2 dx - \sum_{j=1}^{d} \left(\int_{\mathbb{R}^d} x_j |w(x)|^2 dx\right)^2, \tag{3.1}$$

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 $w = \{w_1, \dots, w_m\} \subset L^2(\mathbb{R}^d)$ the **Marzari-Vanderbilt localization functional** is

$$F_{MV}(w) = \sum_{a=1}^{m} F_{MV}(w_a) = \sum_{a=1}^{m} \int_{\mathbb{R}^d} |x|^2 |w_a(x)|^2 dx - \sum_{a=1}^{m} \sum_{j=1}^{d} \left(\int_{\mathbb{R}^d} x_j |w_a(x)|^2 dx\right)^2. \tag{3.2}$$

We emphasize that the above definition of $F_{\mathrm{MV}}(w)$ includes the crucial constraint that the corresponding Bloch functions $\varphi_a(k,\cdot) = (\tilde{\mathcal{U}}_{\mathrm{BF}}\, w_a)(k,\cdot)$, for $a \in \{1, \dots, m\}$, are a Bloch frame, *i.e.* $\{\varphi_1(k,\cdot), \dots, \varphi_m(k,\cdot)\}$ is an orthonormal set in $\mathcal{H}_f$ for each $k \in Y^*$ and

$$\operatorname{Span}_{\mathbb{C}} \{\varphi_1(k,\cdot), \dots, \varphi_m(k,\cdot)\} = P_*(k)(\mathcal{H}_f), \quad \forall k \in Y^*. \tag{3.3}$$

According to Remark 2.5, the latter condition actually implies $w_a \in W^{2,2}(\mathbb{R}^d) = \mathcal{D}(H)$.

Definition 4. *Let $\{P_*(k)\}_{k\in\mathbb{R}^d} \subset \mathcal{B}(\mathcal{H}_{\mathrm{f}})$ be a family of projectors satisfying properties* $(\tilde{\mathrm{P}}_1)$ *and* (P_2), *with* $\dim P_*(k) \equiv m < +\infty$. *A system of* ***maximally localized composite Wannier functions*** *is a global minimizer $\{w_1, \dots, w_m\}$ of the Marzari-Vanderbilt localization* *functional F_{MV} in the set $\mathcal{W}^m := (\mathcal{D}(H) \cap \mathcal{D}(X))^m$, under the constraint that $\{\varphi_1, \ldots, \varphi_m\}$, for $\varphi_a = \tilde{\mathcal{U}}_{\mathrm{BF}} w_a$, is a Bloch frame.*

A natural problem, raised in [MaVa], is the following.

Problem 3.1. Let $\{P_*(k)\}_{k \in \mathbb{R}^d} \subset \mathcal{B}(\mathcal{H}_{\mathrm{f}})$ be a family of projectors satisfying properties $(\tilde{\mathrm{P}}_1)$ and (P_2), with $\dim P_*(k) \equiv m < +\infty$.

(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, in the sense that there exists $\beta > 0$ such that (2.14) holds.

Since the (modified) Bloch-Floquet transform $\tilde{\mathcal{U}}_{\mathrm{BF}} : L^2(\mathbb{R}^d) \to L^2(Y^*; \mathcal{H}_{\mathrm{f}})$ is an isometry and it satisfies $(\tilde{\mathcal{U}}_{BF} X_j g)(k, y) = \mathrm{i} \frac{\partial}{\partial k_j} (\tilde{\mathcal{U}}_{BF} g)(k, y)$, the functional (3.2) can be rewritten in terms of the Bloch frame $\varphi = \{\varphi_1, \ldots, \varphi_m\}$ as
(3.4)
$$\tilde{F}_{MV}(\varphi) = \sum_{a=1}^{m} \sum_{j=1}^{d} \left\{ \int_{Y^*} dk \int_{\mathbb{T}^d} \left| \frac{\partial \varphi_a}{\partial k_j}(k, y) \right|^2 dy - \left(\int_{Y^*} dk \int_{\mathbb{T}^d} \overline{\varphi_a(k, y)}\, i \frac{\partial \varphi_a}{\partial k_j}(k, y)\, dy \right)^2 \right\}.$$

Correspondingly, in view of (2.5), the space $\mathcal{W} = \mathcal{D}(H) \cap \mathcal{D}(X) = \mathcal{D}(H) \cap \mathcal{D}(\langle X \rangle)$ is mapped by the Bloch-Floquet transform into

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

Hereafter, to solve problem (MV_1) for any d, we will make the following

Assumption 1: there exists a Bloch frame $\chi = \{\chi_1, \ldots, \chi_m\} \subset \mathcal{H}_\tau$ such that $\chi_a \in \widetilde{\mathcal{W}}$.

In the case most relevant to us, *i.e.* Schrödinger operators for $d \leq 3$, the previous assumption is automatically satisfied, since Proposition 2.1 and Theorem 2.9 provide the existence of a Bloch frame which is even real-analytic. While this extra regularity is unessential for problem (MV_1), it will be crucial when dealing with (MV_2). Notice that, under the previous assumption, the set of admissible Bloch frames in Definition 4 is non-void, so problem (MV_1) makes sense.

By using the previous Bloch frame, we can lift the functional (3.4) to $W^{1,2}$-maps from $\mathbb{T}^*_d$ to the unitary group $\mathcal{U}(m)$, *i.e.* to Γ^*-periodic maps from $\mathbb{R}^d$ to $\mathcal{U}(m)$. Indeed, given any map $U \in W^{1,2}(\mathbb{T}^*_d, \mathcal{U}(m))$ one defines a Bloch frame $\varphi = \{\varphi_1, \ldots, \varphi_m\} \subset \tilde{\mathcal{W}}$ by setting $\varphi = \chi \cdot U$, *i.e.* $\varphi_a(k, \cdot) = \sum_b \chi_b(k, \cdot)\, U_{b,a}(k)$. Vice versa, if $\varphi = \{\varphi_1, \ldots, \varphi_m\} \subset \tilde{\mathcal{W}}$ is a Bloch frame, then pointwise $\varphi_a(k, \cdot) = \sum_b \chi_b(k, \cdot)\, U_{b,a}(k)$ with $U_{b,a}(k) = \langle \chi_b(k)\,, \varphi_a(k) \rangle$, hence $U \in W^{1,2}(\mathbb{T}^*_d, \mathcal{U}(m))$.

For the given reference frame χ, the functional (3.4) in terms of the gauge U becomes

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

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

$$
(3.6)\qquad \left[A_j(k)\right]_{cb} = \left\langle \chi_c(k,\cdot)\,,\;\frac{\partial \chi_b(k,\cdot)}{\partial k_j}\right\rangle_{\mathcal{H}_f}
$$

When χ is real-analytic, the functions $A_j \in C^\omega(\mathbb{T}_d^*;\mathfrak{u}(m))$ represent the antihermitian connection 1-form induced on the (sub)bundle $\mathcal{E}_*$ by the trivial connection on the bundle $\mathbb{R}^d \times \mathcal{H}_f$.

Moreover,

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

Therefore, problem (MV_1) is equivalent to showing that the r.h.s. of (3.7) is attained. Analogously, in view of Corollary 2.4, 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.

Remark 3.2 (**Rough reference frames, as in numerical simulations**)**.** When reformulating problem (MV_1) in terms of the functional $\tilde{F}_{MV}(U;\chi)$ the regularity of the reference frame χ plays no essential role, provided χ is in $\tilde{\mathcal{W}}$. Indeed, in view of (3.7), the infimum on the r.h.s does not depend on the choice of χ. Moreover, if for a particular choice of χ the infimum is attained at U, then for another choice $\tilde{\chi}\subset\tilde{\mathcal{W}}$ the infimum is attained at $\tilde{U}=V\,U$, where $\chi=\tilde{\chi}\cdot V$. The matrix V, defined by $V_{b,a}(k)=\langle\tilde{\chi}_b(k)\,,\,\chi_a(k)\rangle$, is in $W^{1,2}(\mathbb{T}_d^*;\mathcal{U}(m))$, hence $\tilde{U}$ is also in $W^{1,2}(\mathbb{T}_d^*;\mathcal{U}(m))$. This observation justifies the fact that a minimizer (whenever it exists) can be evaluated starting from any reference Bloch frame $\chi\subset\tilde{\mathcal{W}}$, even a discontinuous one, as it happens in numerical simulations.

Remark 3.3 (**Minimizing over smooth gauges**)**.** To compute the infimum of $\tilde{F}_{MV}(U;\chi)$ it is sufficient to consider smooth change of gauges. More precisely, for $d\le 3$ and for any fixed Bloch frame $\chi\subset\tilde{\mathcal{W}}$ one has

$$
\inf\left\{\tilde{F}_{MV}(U;\chi)\;:\;U\in W^{1,2}(\mathbb{T}_d^*;\mathcal{U}(m))\right\} = \inf\left\{\tilde{F}_{MV}(U;\chi)\;:\;U\in C^\infty(\mathbb{T}_d^*;\mathcal{U}(m))\right\}.
$$

As a consequence, in numerical implementations, to compute the above infimum one can let U vary in any set S such that $C^\infty(\mathbb{T}_d^*;\mathcal{U}(m))\subset S\subset W^{1,2}(\mathbb{T}_d^*;\mathcal{U}(m))$.

This result follows from the strong density of smooth maps $C^\infty(\mathbb{T}_d^*;\mathcal{U}(m))\subset W^{1,2}(\mathbb{T}_d^*;\mathcal{U}(m))$ for $d\le 3$. If $d=2$ the latter claim is essentially the approximation by convolution followed by the nearest-point projection onto the unitary group; if $d=3$, the claim follows from the fact that the homotopy group $\pi_2(\mathcal{U}(m))$ is trivial and from the fact that $\mathbb{T}_3^*$ has the 1-extension property with respect to $\mathcal{U}(m)$, see [HL, Theorem 1.3 and Section 5].

3.1. **Existence of minimizers.** The following results shows that the right hand side in (3.7) is attained. The proof is a simple modification of the direct method in the calculus of variations, in order to handle a natural invariance of the functional (3.2). Indeed, if $\{w_1, \dots, w_m\}$ are composite Wannier functions satisfying (3.3) and $\{\gamma_1, \dots, \gamma_m\} \subset \Gamma$, then

$$F_{MV}(w_1, \dots, w_m) = F_{MV}(\tilde{w}_1, \dots, \tilde{w}_m) , \quad \tilde{w}_a(x) = w_a(x + \gamma_a) , \quad 1 \le a \le m . \tag{3.8}$$

Moving to Bloch functions, we have $\tilde{\varphi}_a(k, \cdot) \equiv \left(\tilde{\mathcal{U}}_{BF}\, \tilde{w}_a\right)(k, \cdot) = e^{ik\gamma_a} \left(\tilde{\mathcal{U}}_{BF}\, w_a\right)(k, \cdot)$, so that $\{\tilde{\varphi}_1(k, \cdot), \dots, \tilde{\varphi}_m(k, \cdot)\}$ is still orthonormal in $\mathcal{H}_f$ and (3.3) holds. Correspondingly, the functional (3.5) has the invariance

$$\tilde{F}_{MV}(U; \chi) = \tilde{F}_{MV}(\tilde{U}; \chi) , \quad \tilde{U}(k) = \operatorname{diag}\left(e^{ik\gamma_a}\right) U(k) . \tag{3.9}$$

Theorem 3.4. *Let $\{P_*(k)\}_{k \in \mathbb{R}^d} \subset \mathcal{B}(\mathcal{H}_{\mathrm{f}})$ be a family of orthogonal projectors satisfying properties $(\tilde{\mathrm{P}}_1)$ and (P_2), with $\dim P_*(k) \equiv m$. Assume that there exists a Bloch frame $\chi \subset \tilde{\mathcal{W}}$. Then there exists $U \in W^{1,2}(\mathbb{T}_d^*; \mathcal{U}(m))$ which is a minimizer on $W^{1,2}(\mathbb{T}_d^*; \mathcal{U}(m))$ of the localization functional $\tilde{F}_{MV}(\cdot, \chi)$ defined by (3.5).*

Proof. Note that $\tilde{F}(\cdot; \chi)$ is nonnegative, because of (3.7) and (3.2). Note also that $E(U) = \sum_{j=1}^d \int_{\mathbb{T}_d^*} \frac{1}{2} \operatorname{tr}\left(\frac{\partial U^*}{\partial k_j}(k) \frac{\partial U}{\partial k_j}(k)\right)$ is the standard Dirichlet integral so it is (sequentially) weakly lower semicontinuous on $W^{1,2}$. Thus $\tilde{F}(\cdot; \chi)$ is weakly lower semicontinuous in $W^{1,2}$, because the first term in (3.5) is, up to a constant factor, $E(\cdot)$ and the other terms are clearly weakly continuous (because of the compact embedding $W^{1,2}(\mathbb{T}_d^*) \hookrightarrow L^2(\mathbb{T}_d^*)$). In order to apply the direct method it remains to show that the functional is coercive, so that there exists a minimizing sequence which is bounded in $W^{1,2}(\mathbb{T}_d^*; \mathcal{U}(m))$. However, coercivity clearly fails because of the natural invariance of $\tilde{F}(\cdot; \chi)$ given by (3.9) (the $W^{1,2}$-norm of $\tilde{U}$ can be made arbitrarily large as $|\gamma_a| \to \infty$).

In order to fix the argument it is enough to take advantage of this invariance in the form (3.8). Indeed, for any admissible U we can choose $\gamma_1, \dots, \gamma_m$ so that the corresponding $\tilde{U}$, defined as in (3.9), gives the same value of $\tilde{F}_{MV}(\cdot; \chi)$ but in such a way that the corresponding Wannier functions $\{w_a\}$ satisfy $\sum_{j=1}^d \left|\int_{\mathbb{R}^d} x_j |w_a(x)|^2 dx\right| \le C$ for some absolute constant $C > 0$ independent of U. Thus, if along a sequence $\{U_n\}$ the functional $\tilde{F}_{MV}$ is bounded, up to a suitable choice of the translation parameters $\{\gamma_a^n\}$ we have a uniform bound for the modified sequence $\{\tilde{U}_n\}$ in $W^{1,2}$ (the third line in (3.5) is now bounded by $C^2 md$ and the first two are easily seen to be equivalent to the Dirichlet energy up to additive and multiplicative constants depending only on A, C and m).

Then, up to subsequences, $\tilde{U}_n$ weakly converges to some $U \in W^{1,2}(\mathbb{T}_d^*; \mathcal{U}(m))$ which is a minimizer. □

3.2. **The Euler-Lagrange equations.** In this subsection we derive the Euler-Lagrange equations corresponding to the functional (3.5). To our knowledge, these equations are new in the literature. We consider the unitary group $\mathcal{U}(m)$ as isometrically embedded into the space $M_m(\mathbb{C})$ with the standard real Euclidean product $\langle A\,,\,B\rangle = \mathrm{Re}\,\mathrm{tr}(A^*B)$. Recall that $\mathcal{U}(m)$ is a compact real Lie group, the induced metric is biinvariant, its Lie algebra is given by the real vector space of complex antihermitian matrices and it has dimension m^2.

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 neiborhood $\mathcal{O}$ of $\mathcal{U}(m)$ in $M_m(\mathbb{C})$ there is a well defined smooth nearest point projection map $\Pi : \mathcal{O} \to \mathcal{U}(m)$, so we can consider the induced variations

$$U_\varepsilon(k) := \Pi(U(k)+\varepsilon\varphi(k)) = U(k)\left(\mathbb{I} + \varepsilon\frac{1}{2}\left[U^{-1}(k)\varphi(k) - (U^{-1}(k)\varphi(k))^*\right]\right) + o(\varepsilon)\,. \tag{3.10}$$

Simple calculations on each term in (3.5) yield

$$\left.\frac{d}{d\varepsilon}\right|_{\varepsilon=0} \int_{\mathbb{T}^*_d} \mathrm{tr}\left(\frac{\partial U^*_\varepsilon}{\partial k_j}(k)\frac{\partial U_\varepsilon}{\partial k_j}(k)\right) dk = 2\int_{\mathbb{T}^*_d} \mathrm{tr}\left[\frac{\partial \varphi^*}{\partial k_j}(k)\frac{\partial U}{\partial k_j}(k) + \varphi^*(k)\frac{\partial U}{\partial k_j}(k)U^{-1}(k)\frac{\partial U}{\partial k_j}(k)\right] dk\,, \tag{3.11}$$

$$\left.\frac{d}{d\varepsilon}\right|_{\varepsilon=0} \int_{\mathbb{T}^*_d} \mathrm{tr}\left[\left(U_\varepsilon(k)\frac{\partial U^*_\varepsilon}{\partial k_j}(k) - \frac{\partial U_\varepsilon}{\partial k_j}(k)U^*_\varepsilon(k)\right)A_j(k)\right] dk = \tag{3.12}$$

$$= 2\int_{\mathbb{T}^*_d} \mathrm{tr}\left[\varphi^*(k)\left\{\frac{\partial U}{\partial k_j}(k)U^{-1}(k)A_j(k)U(k) - \frac{\partial A_j}{\partial k_j}(k)U(k) - A_j(k)\frac{\partial U}{\partial k_j}(k)\right\}\right] dk\,,$$

and

$$\left.\frac{d}{d\varepsilon}\right|_{\varepsilon=0} \sum_{a=1}^m \left(\int_{\mathbb{T}^*_d}\left[U^*_\varepsilon(k)\left(\frac{\partial U_\varepsilon}{\partial k_j}(k) + A_j(k)U_\varepsilon(k)\right)\right]_{aa} dk\right)^2 = \tag{3.13}$$

$$= 2\int_{\mathbb{T}^*_d} \mathrm{tr}\left[\varphi^*(k)\left\{-\left(\frac{\partial U}{\partial k_j}(k) + A_j(k)U(k)\right)G^j + U(k)G^jU^{-1}(k)\left(\frac{\partial U}{\partial k_j}(k) + A_j(k)U(k)\right)\right\}\right] dk\,.$$

Here the constant (purely imaginary) diagonal matrices $\{G^j\} \subset M_m(\mathbb{C})$ are defined as $G^j = \mathrm{diag}\left(\int_{\mathbb{T}^*_d} U^*(k)\left[\frac{\partial U}{\partial k_j}(k) + A_j(k)U(k)\right] dk\right)$, where $[\mathrm{diag}\, M]_{ab} = M_{aa}\delta_{ab}$.

Thus 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 to the Euler-Lagrange equations

$$\begin{aligned} -\Delta U + \sum_{j=1}^d \frac{\partial U}{\partial k_j}U^{-1}\frac{\partial U}{\partial k_j} + \sum_{j=1}^d\left[\frac{\partial U}{\partial k_j}U^{-1}A_jU - \frac{\partial A_j}{\partial k_j}U - A_j\frac{\partial U}{\partial k_j}\right] + \\ + \sum_{j=1}^d\left[-\left(\frac{\partial U}{\partial k_j} + A_jU\right)G^j + UG^jU^{-1}\left(\frac{\partial U}{\partial k_j} + A_jU\right)\right] = 0\,. \end{aligned} \tag{3.14}$$

4. Continuity of minimizers

The goal of this section is to show that a change of gauge $U \in W^{1,2}(\mathbb{T}^*_d;\mathcal{U}(m))$ which minimizes the functional (3.5) is continuous, whenever χ is real-analytic. This result will be true if $m = 1$ for any d, if $1 \le d \le 2$ for any m and for $d = 3$ under the restriction $2 \le m \le 3$. The proofs in the three cases are different. The first case, treated in the next proposition, is the simplest and it gives even real-analiticity. In order to deal with the other two cases, we will need a dimension dependent argument which will occupy the rest of the section. Note that in the first two cases continuity holds for any solution of the Euler Lagrange equations. In contrast, in the three dimensional case continuity relies on energy minimality in an essential way.

To deal with the regularity of the minimizers, we make the following assumption which, as already noticed after stating the weaker Assumption 1, is automatically satisfied for $d \le 3$ or $m = 1$ (compare Theorem 2.9).

Assumption 2: there exists a Bloch frame $\chi = \{\chi_1, \dots, \chi_m\} \subset \mathcal{H}_\tau$ such that $\chi_a \in C^\omega(\mathbb{R}^d, \mathcal{H}_{\mathrm{f}})$ for every $a \in \{1, \dots, m\}$.

Proposition 4.1. *Let $d = 1$ and $m \ge 1$, or $d \ge 1$ and $m = 1$. Let $U \in W^{1,2}(\mathbb{T}^*_d;\mathcal{U}(m))$ be a weak solution to equation* (3.14)*. Then U is real-analytic.*

Proof. Assume $d = 1$. Since $U \in W^{1,2}(\mathbb{T}^*_d,\mathcal{U}(m))$, then (3.14) yields $\frac{d^2}{dk^2}U \in L^1$. Thus $U \in W^{2,1}$. Therefore U is in C^1 by Sobolev embedding, and (3.14) implies $U \in C^2$. Analogously, if $U \in C^{n+1}$ solves (3.14), $n \ge 1$, then $U \in C^{n+2}$, so by induction $U \in C^\infty$. Finally, since $A_j \in C^\omega$ for all j, by the standard ODE regularity theory one obtains $U \in C^\omega$.

Now assume $m = 1$. Since $\mathcal{U}(1)$ is abelian the equation (3.14) reduces to

$$- \Delta U + \sum_{j=1}^{d} \frac{\partial U}{\partial k_j} U^{-1} \frac{\partial U}{\partial k_j} = \left(\sum_{j=1}^{d} \frac{\partial A_j}{\partial k_j} \right) U \, . \tag{4.1}$$

Recall that in any sufficiently small ball $B \subset \mathbb{T}^*_d$ we have $U(k) = e^{if(k)}$ for some $f \in W^{1,2}(B;\mathbb{R})$ (see [BZ]). Thus, equation (4.1) reads $\Delta f = i \sum_{j=1}^{d} \frac{\partial A_j}{\partial k_j} \in C^\omega(B;\mathbb{R})$, because the matrices in the Berry connection are antihermitian and real-analytic. Since the Laplacian is analytic-hypoelliptic we conclude $f \in C^\omega(B)$ and in turn $U \in C^\omega(\mathbb{T}^*_d;\mathcal{U}(1))$ since the ball B can be choosen arbitrarily. □

4.1. **Continuity in the two dimensional case.**

We are going to prove continuity of any weak solutions to (3.14) in the case $d = 2$. The argument here is just sketched, since, up to a standard localization argument, it essentially follows the proof of continuity for weakly harmonic maps from a two dimensional domain into spheres (see e.g. [LW1], Chapter III, Section 3.2 pag. 57-61).

We start with the following auxiliary result which is a straightforward consequence of [CLMS].

Lemma 4.2. *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*

$$\Delta U = \sum_{j=1}^{d} \frac{\partial U}{\partial k_j} \tilde{B}^j + \tilde{f} \qquad \text{and } U^{-1} \tilde{f} \in L^p(\mathbb{T}_d^*; \mathfrak{u}(m)) \tag{4.2}$$

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

Proof. We have

$$\Delta U_{a,c} = \sum_{b=1}^{m} \sum_{j=1}^{d} \frac{\partial U_{ab}}{\partial k_j} \tilde{B}^j_{bc} + \tilde{f}_{ac} = \sum_{b=1}^{m} E_{ab} \cdot \tilde{B}_{ab} + \tilde{f}_{ac} \,,$$

where for fixed a, b, c the vector fields $\tilde{B}_{bc}$ and $E_{ab} = \nabla U_{ab}$ are in L^2 and satisfy $\operatorname{div} \tilde{B}_{bc} = 0$ and $\operatorname{curl} E_{ab} = 0$ in the sense of distributions. According to [CLMS], we have $E_{ab} \cdot \tilde{B}_{bc} \in \mathcal{H}^1_{\text{loc}}(\mathbb{T}_d^*)$ and $\tilde{f}_{ac} \in \mathcal{H}^1_{\text{loc}}(\mathbb{T}_d^*)$, *i.e.* the right hand side of (4.2) is in the local Hardy space $\mathcal{H}^1_{\text{loc}}(\mathbb{T}_d^*) \subset L^1(\mathbb{T}_d^*)$. Here $g \in \mathcal{H}^1_{\text{loc}}(\mathbb{T}_d^*)$ means that $g \in \mathcal{H}^1_{\text{loc}}(B)$ for every sufficiently small ball $B \subset \mathbb{T}_d^*$ (namely, for every ball with radius smaller than the injectivity radius of the exponential map). For the definition and the basic properties of $\mathcal{H}^1_{\text{loc}}(\mathbb{R}^d)$ we refer to [St, Chapter 3]. Thus the conclusion follows from [LW1, Theorem 3.2.4]. □

Based on the previous lemma we have the following intermediate result.

Proposition 4.3. *Let $d \geq 2$, $m \geq 2$ and $U \in W^{1,2}(\mathbb{T}_d^*; \mathcal{U}(m))$. If U is a weak solution to*

$$\Delta U = \sum_{j=1}^{d} \frac{\partial U}{\partial k_j} U^{-1} \frac{\partial U}{\partial k_j} + f \qquad \text{and } U^{-1} f \in L^2(\mathbb{T}_d^*; \mathfrak{u}(m)), \tag{4.3}$$

then $U \in W^{2,1}(\mathbb{T}_d^*; \mathcal{U}(m))$. In particular, if $d = 2$ then $U \in C^0(\mathbb{T}_2^*; \mathcal{U}(m))$.

Proof. If we set $B^j = \frac{1}{2}\left(U^* \frac{\partial U}{\partial k_j} - \frac{\partial U^*}{\partial k_j} U\right)$ then $B^j \in L^2(\mathbb{T}_d^*; \mathfrak{u}(m))$ for $j \in \{1, \dots, d\}$, U is a weak solution to (4.2) but $\operatorname{div} B = \frac{1}{2}(U^* f - f U^*) \neq 0$ in $\mathcal{D}'(\mathbb{T}_d^*)$. Note that $\operatorname{div} B \in L^2_0(\mathbb{T}_d^*; \mathfrak{u}(m))$, the space of zero-mean L^2-integrable functions, hence $\Delta^{-1} \operatorname{div} B \in W^{2,2}(\mathbb{T}_d^*; \mathfrak{u}(m))$ by elliptic regularity and if we set

$$\tilde{B} = B - \nabla \Delta^{-1} \operatorname{div} B \,, \qquad \tilde{f} = f + \nabla U \cdot \nabla \Delta^{-1} \operatorname{div} B \,,$$

then $\tilde{B}$, $\tilde{f}$ and U satisfy the assumptions of Lemma 4.2 by Sobolev embedding (for some $p > 1$ depending only on d), hence we obtain $U \in W^{2,1}(\mathbb{T}_d^*; \mathcal{U}(m))$. Finally, if $d = 2$ the improved Sobolev embeddings into Lorentz spaces yield $\nabla U \in L^{2,1}$ and in turn $U \in C^0$ (see [LW1], Theorem 3.2.7 and 3.2.8 respectively). □

Going back to equation (3.14) we have the following important consequence

Corollary 4.4. *Let $d = 2$, $m \geq 2$ and $U \in W^{1,2}(\mathbb{T}_2^*; \mathcal{U}(m))$ a weak solution to equation (3.14). Then $U \in W^{2,1}(\mathbb{T}_2^*; \mathcal{U}(m))$ and $U \in C^0(\mathbb{T}_2^*; \mathcal{U}(m))$.*

Proof. If $U \in W^{1,2}(\mathbb{T}_2^*;\mathcal{U}(m))$ is a weak solution to equation (3.14) then U satisfies also (4.3) for a suitable f depending on U. Here $U^{-1}f \in L^2(\mathbb{T}_2^*;\mathfrak{u}(m))$ because of the regularity property of U and the Berry connection $A_j \in C^\omega(\mathbb{T}_2^*,\mathfrak{u}(m))$, in view of the structure of equation (3.14). Thus, the conclusion follows from Proposition 4.3. □

4.2. **Continuity in the three dimensional case.** The goal of this subsection is to show that if $d = 3$ then minimizers of the localization functional (3.5) are continuous, at least if $m \leq 3$. Roughly speaking the idea is to prove that at smaller and smaller scales minimizers look like minimizing harmonic maps into the unitary group $\mathcal{U}(m)$ which are degree-zero homogeneous. Since the latter are constant, at least for $m \leq 3$ (see Corollary A.10 below), then the former are continuous at a sufficiently small scale. All the techniques in this section are inspired by the regularity theory for minimizing harmonic maps (see [SU1], [Si] and [LW1]).

The first condition we need to study minimizers at small scales is the stationarity condition with respect to inner variations.

Lemma 4.5. *Let $d \geq 3$ and let $U \in W^{1,2}(\mathbb{T}_d^*;\mathcal{U}(m))$ be a minimizer of (3.5). For each $1 \leq j \leq d$ define constant diagonal matrices $G^j = \operatorname{diag}\int U^*(\frac{\partial U}{\partial k_j} + A_j U)dk$. Let $\Phi \in C^\infty(\mathbb{T}_d^*;\mathbb{R}^d)$ be a smooth vector field and $\Psi_\varepsilon(k) = k + \varepsilon\,\Phi(k)$ be a family of diffeomorphisms (for ε small enough). Then*

$$\frac{d}{d\varepsilon}\bigg|_{\varepsilon=0} \tilde{F}_{MV}(U\circ\Psi_\varepsilon;\chi) = \sum_{j,c}\int \frac{\partial \Phi^c}{\partial k_c}\operatorname{tr}\left[-\frac{\partial U^*}{\partial k_j}\frac{\partial U}{\partial k_j} + 2\frac{\partial U}{\partial k_j}U^*A_j - 2G^jU^*\left(\frac{\partial U}{\partial k_j} + A_jU\right)\right] +$$
$$\sum_{j,c}\int \frac{\partial \Phi^c}{\partial k_j}\operatorname{tr}\left[\frac{\partial U^*}{\partial k_c}\frac{\partial U}{\partial k_j} + \frac{\partial U^*}{\partial k_j}\frac{\partial U}{\partial k_c} - 2\frac{\partial U}{\partial k_c}U^*A_j + 2G^jU^*\frac{\partial U}{\partial k_c}\right] +$$
$$\sum_{j,c}\int \Phi^c\operatorname{tr}\left[2\frac{\partial U}{\partial k_j}\frac{\partial A_j}{\partial k_c} - 2G^jU^*\frac{\partial A_j}{\partial k_c}U\right]. \tag{4.4}$$

Proof. First note that $\det D\Psi_\varepsilon^{-1}(k) = 1 - \varepsilon\operatorname{div}\Phi + o(\varepsilon)$ uniformly on $\mathbb{T}_d^*$. As a consequence the change of variable and the chain rule give

$$\frac{d}{d\varepsilon}\bigg|_{\varepsilon=0}\int f(\Psi_\varepsilon(k))g(k)dk = -\int f(k)g(k)\operatorname{div}\Phi(k)dk - \sum_c\int f(k)\frac{\partial g}{\partial k_c}(k)\Phi^c(k)dk\,. \tag{4.5}$$

for any $f \in L^1$ and for any $g \in C^1$. Now we set $U_\varepsilon(k) = U\circ\Psi_\varepsilon(k)$, so that

$$\frac{\partial U_\varepsilon}{\partial k_j}(k) = \sum_c \frac{\partial U}{\partial k_c}(\Psi_\varepsilon(k))\frac{\partial \Psi_\varepsilon^c(k)}{\partial k_j} = \sum_c \frac{\partial U}{\partial k_c}(\Psi_\varepsilon(k))(\delta_j^c + \varepsilon\frac{\partial \Phi^c(k)}{\partial k_j})\,. \tag{4.6}$$

Thus, a repeated application of (4.5) and (4.6) gives

$$\frac{d}{d\varepsilon}\bigg|_{\varepsilon=0}\sum_j\int\operatorname{tr}\left[\frac{\partial U_\varepsilon^*}{\partial k_j}\frac{\partial U_\varepsilon}{\partial k_j}\right]dk = -\sum_j\int\operatorname{div}\Phi(k)\,\operatorname{tr}\left[\frac{\partial U_\varepsilon^*}{\partial k_j}\frac{\partial U_\varepsilon}{\partial k_j}\right] + \tag{4.7}$$
$$\sum_{j,c}\int\frac{\partial \Phi^c(k)}{\partial k_j}\operatorname{tr}\left[\frac{\partial U^*}{\partial k_c}\frac{\partial U}{\partial k_j} + \frac{\partial U^*}{\partial k_j}\frac{\partial U}{\partial k_c}\right],$$

$$\left.\frac{d}{d\varepsilon}\right|_{\varepsilon=0} \sum_j \int \operatorname{tr}\left[\left(U_\varepsilon \frac{\partial U_\varepsilon^*}{\partial k_j} - \frac{\partial U_\varepsilon}{\partial k_j} U_\varepsilon^*\right) A_j(k)\right] dk = \tag{4.8}$$

$$= -\sum_{j,c} \int \operatorname{tr}\left[\left(U \frac{\partial U^*}{\partial k_j} - \frac{\partial U}{\partial k_j} U^*\right)\left(A_j(k) \frac{\partial \Phi^c}{\partial k_c} + \frac{\partial A_j}{\partial k_c} \Phi^c\right)\right] dk +$$

$$+ \sum_{j,c} \int \operatorname{tr}\left[\left(U \frac{\partial U^*}{\partial k_c} - \frac{\partial U}{\partial k_c} U^*\right) A_j(k) \frac{\partial \Phi^c}{\partial k_j}\right] dk.$$

Similarly, taking the definition of G^j into account, one has

$$\left.\frac{d}{d\varepsilon}\right|_{\varepsilon=0} \sum_{j,a} \left(\int \left[U_\varepsilon^* \left(\frac{\partial U_\varepsilon}{\partial k_j} + A_j U_\varepsilon\right)\right]_{aa}\right)^2 = \tag{4.9}$$

$$= \sum_{j,c} \int \operatorname{tr}\left[-2G^j U^* \left(\frac{\partial U}{\partial k_j} + A_j U\right) \frac{\partial \Phi^c}{\partial k_c} + 2G^j U^* \frac{\partial U}{\partial k_c} \frac{\partial \Phi^c}{\partial k_j} - 2G^j U^* \frac{\partial A_j}{\partial k_c} U \Phi^c\right].$$

Combining (4.7), (4.8) and (4.9) with the definition of (3.5) and reorganizing the sum we easily have (4.4). □

The first consequence we obtain is a sort of perturbed monotonicity formula (in the spirit of the monotonicity formula for almost harmonic maps; see [Mos], Chapter 4).

Proposition 4.6. *Let $d \geq 3$ and let $U \in W^{1,2}(\mathbb{T}_d^*; \mathcal{U}(m))$ be a minimizer of the localization functional (3.5). Then there exist $C > 0$ and $\bar{R} > 0$ such that for each $k_0 \in \mathbb{T}_d^*$ and for each R_1, R_2 with $0 < R_1 \leq R_2 \leq \bar{R}$ we have*

$$\frac{1}{R_1^{d-2}} \int_{B_{R_1}(k_0)} |\nabla U|^2 + \int_{R_1 < |k-k_0| < R_2} \frac{2}{|k-k_0|^{d-2}} \left|\frac{\partial U}{\partial r}\right|^2 \leq 2CR_2 + (1 + 2CR_2) \frac{1}{R_2^{d-2}} \int_{B_{R_2}(k_0)} |\nabla U|^2. \tag{4.10}$$

As a consequence, the function $R^{2-d} \int_{B_R(k_0)} |\nabla U|^2 dk$ has a limit and $\int_{B_R(k_0)} |\partial_r U|^2 |k-k_0|^{2-d} dk$ is finite and vanishes as $R \to 0^+$.

Proof. Clearly by translation invariance it suffices to consider the case $k_0 = 0$. We take $h \in C^\infty(\mathbb{R})$ an increasing function such that $h(t) \equiv 0$ for $t < 0$ and $h(t) \equiv 1$ for $t \geq 1$. If we take $\Phi(k) = k\, h(R - |k|)$ in (4.4) we have $\operatorname{div} \Phi(k) = d\, h(R-|k|) - |k| h'(R-|k|)$ ($d \in \mathbb{N}$ is the dimension) and

$$\frac{\partial \Phi^c}{\partial k_j} = \delta_j^c h - \frac{k_c k_j}{|k|} h', \quad \sum_c \frac{\partial U}{\partial k_c} \frac{\partial \Phi^c}{\partial k_j} = \frac{\partial U}{\partial k_j} h - k_j \frac{\partial U}{\partial r} h', \quad \sum_c \frac{\partial A_j}{\partial k_c} \Phi^c = |k| \frac{\partial A_j}{\partial r} h. \tag{4.11}$$

Combining (4.4) and (4.11) we get

$$0 = \sum_j \int_{B_R} (dh - |k| h') \operatorname{tr}\left[-\frac{\partial U^*}{\partial k_j} \frac{\partial U}{\partial k_j} + 2 \frac{\partial U}{\partial k_j} U^* A_j - 2G^j U^* \left(\frac{\partial U}{\partial k_j} + A_j U\right)\right] +$$

$$- \sum_j \int_{B_R} k_j \operatorname{tr}\left[\frac{\partial U^*}{\partial r} \frac{\partial U}{\partial k_j} + \frac{\partial U^*}{\partial k_j} \frac{\partial U}{\partial r} - 2 \frac{\partial U}{\partial r} U^* A_j + 2G^j U^* \frac{\partial U}{\partial r}\right] h' +$$

$$+2\sum_j\int_{B_R}\operatorname{tr}\left[\frac{\partial U^*}{\partial k_j}\frac{\partial U}{\partial k_j}-\frac{\partial U}{\partial k_j}U^*A_j+G^jU^*\frac{\partial U}{\partial k_j}+|k|\frac{\partial U}{\partial k_j}\frac{\partial A_j}{\partial r}-|k|G^jU^*\frac{\partial A_j}{\partial r}U\right]h\,. \tag{4.12}$$

Passing to the limit as $h\to\chi_{\{t>0\}}$, as in [Si, Chapter 2], yields

$$0=\sum_j\int_{B_R}\operatorname{tr}\left[(2-d)\frac{\partial U^*}{\partial k_j}\frac{\partial U}{\partial k_j}\right]+R\sum_j\int_{\partial B_R}\operatorname{tr}\left[\frac{\partial U^*}{\partial k_j}\frac{\partial U}{\partial k_j}\right]-2R\int_{\partial B_R}\operatorname{tr}\left[\frac{\partial U^*}{\partial r}\frac{\partial U}{\partial r}\right] \tag{4.13}$$

$$-\sum_j\int_{\partial B_R}|k|\operatorname{tr}\left[2\frac{\partial U}{\partial k_j}U^*A_j-2G^jU^*\left(\frac{\partial U}{\partial k_j}+A_jU\right)-2\frac{k_j}{|k|}\frac{\partial U}{\partial r}U^*A_j+2\frac{k_j}{|k|}G^jU^*\frac{\partial U}{\partial r}\right]+$$

$$2\sum_j\int_{B_R}\operatorname{tr}\left[(d-1)\left(\frac{\partial U}{\partial k_j}U^*A_j-G^jU^*\frac{\partial U}{\partial k_j}\right)-dG^jU^*A_jU+|k|\frac{\partial U}{\partial k_j}\frac{\partial A_j}{\partial r}-|k|G^jU^*\frac{\partial A_j}{\partial r}U\right].$$

Note that $R^{d-1}\frac{d}{dR}\left(R^{2-d}\int_{B_R}f\right)=(2-d)\int_{B_R}f-R\int_{\partial B_R}f$ for any integrable function f and for a.e. $R>0$. Thus, dividing in (4.13) by R^{d-1} and integrating on $[R_1,R_2]$ we have

$$\frac{1}{R_1^{d-2}}\int_{B_{R_1}}|\nabla U|^2+\int_{R_1<|k|<R_2}\frac{2}{|k|^{d-2}}\left|\frac{\partial U}{\partial r}\right|^2=\frac{1}{R_2^{d-2}}\int_{B_{R_2}}|\nabla U|^2 \tag{4.14}$$

$$+\int_{R_1<|k|<R_2}V(k,U)+\int_{R_1}^{R_2}\frac{dR}{R^{d-1}}\int_{B_R}W(k,U)\,,$$

where

$$V(k,U)=2|k|^{2-d}\operatorname{tr}\left[-\frac{\partial U}{\partial k_j}U^*A_j+G^jU^*\left(\frac{\partial U}{\partial k_j}+A_jU\right)+\frac{k_j}{|k|}\frac{\partial U}{\partial r}U^*A_j-\frac{k_j}{|k|}G^jU^*\frac{\partial U}{\partial r}\right]$$

and

$$W(k,U)=2\operatorname{tr}\left[(d-1)\left(\frac{\partial U}{\partial k_j}U^*A_j-G^jU^*\frac{\partial U}{\partial k_j}\right)-dG^jU^*A_jU+|k|\frac{\partial U}{\partial k_j}\frac{\partial A_j}{\partial r}-|k|G^jU^*\frac{\partial A_j}{\partial r}U\right]$$

Notice that the first line in (4.14) is the usual monotonicity identity for harmonic maps from $\mathbb{T}_d^*$ with values into $\mathcal{U}(m)$. To estimate the extra terms in (4.14), observe that for fixed matrices G^j we have $|V(k,U)|\le C|k|^{2-d}(1+|\nabla U|)$ where the constant depends on the C^0 norm of the Berry connection matrices A_j. Similarly we have $|W(k,U)|\le C(1+|\nabla U|)$ where the constant depends only on the C^1 norm of the Berry connection matrices. Thus, if $l_0\ge 1$ is an integer and $R_1\ge 2^{-l_0}R_2$, $R_2\le 1$ and $0<\delta=R_2\le 1$ we have (writing $\fint_B$ for $\frac{1}{|B|}\int_B$)

$$\int_{R_1<|k|<R_2}|V(k,U)|\le C\int_{R_1<|k|<R_2}|k|^{2-d}(1+|\nabla U|)\le$$

$$CR_2^2+C\sum_{l=0}^{l_0-1}\int_{2^{-l-1}R_2<|k|<2^{-l}R_2}|k|^{2-d}|\nabla U|\le CR_2^2+C\sum_{l=0}^{l_0-1}2^{-2l}R_2^2\sqrt{\fint_{B_{2^{-l}R_2}}|\nabla U|^2}\le$$

$$CR_2^2+\delta\sup_{r\in[2^{-l_0}R_2,R_2]}\frac{1}{r^{d-2}}\int_{B_r}|\nabla U|^2+C\delta^{-1}R_2^2\le CR_2\left(1+\sup_{r\in[2^{-l_0}R_2,R_2]}\frac{1}{r^{d-2}}\int_{B_r}|\nabla U|^2\right).$$

On the other hand, a similar estimate with $\delta = \delta_l = 2^{-l} R_2$ gives

$$\int_{R_1}^{R_2} \frac{dR}{R^{d-1}} \int_{B_R} |W(k,U)| \leq C R_2^2 + \int_{R_1}^{R_2} \frac{dR}{R^{d-1}} \int_{B_R} |\nabla U| \leq C R_2^2 +$$

$$+ C \sum_{l=0}^{l_0-1} \int_{2^{-l-1}R_2}^{2^{-l}R_2} \frac{dR}{R} \frac{1}{R^{d-2}} \int_{B_R} |\nabla U| \leq C \left[R_2^2 + \left(\sum_{l=0}^{l_0-1} \delta_l \right) \sup_{r \in [2^{-l_0} R_2, R_2]} \frac{1}{r^{d-2}} \int_{B_r} |\nabla U|^2 \right.$$

$$\left. + \sum_{l=0}^{l_0-1} \frac{1}{\delta_l} R^2 |_{2^{-l-1}R_2}^{2^{-l}R_2} \right] \leq C R_2 \left(1 + \sup_{r \in [2^{-l_0} R_2, R_2]} \frac{1}{r^{d-2}} \int_{B_r} |\nabla U|^2 \right).$$

Combining the two estimates above we obtain

(4.15)

$$\int_{R_1 < |k| < R_2} |V(k,U)| + \int_{R_1}^{R_2} \frac{dR}{R^{d-1}} \int_{B_R} |W(k,U)| \leq C R_2 \left(1 + \sup_{r \in [2^{-l_0} R_2, R_2]} \frac{1}{r^{d-2}} \int_{B_r} |\nabla U|^2 \right)$$

Going back to (4.14), if $R_2 \leq \bar{R} := \min\{1, \frac{1}{2} C^{-1}\}$ is fixed, taking the supremum over $R_1 \in [2^{-l_0} R_2, R_2]$ and estimating the right hand side using (4.15) one easily obtains

$$\sup_{r \in [2^{-l_0} R_2, R_2]} \frac{1}{r^{d-2}} \int_{B_r} |\nabla U|^2 \leq 1 + 2 \frac{1}{R_2^{d-2}} \int_{B_{R_2}} |\nabla U|^2 .$$

Combining (4.14), (4.15) and the previous inequality we finally obtain (4.10). Letting $R_1 \to 0$ in (4.10) we see that $R^{2-d} \int_{B_R} |\nabla U|^2 dk$ is bounded and $\int_{B_R} |\partial_r U|^2 |k|^{2-d} dk$ is finite and therefore vanishing as $R \to 0^+$. As a consequence, letting $R_1 \to 0$ and $R_2 \to 0$ in (4.10), it is straightforward to see that $R^{2-d} \int_{B_R} |\nabla U|^2 dk$ has a limit as $R \to 0$. □

Remark 4.7. A simple consequence of (4.10) is that if $\lim_{R \to 0} R^{2-d} \int_{B_R(k_0)} |\nabla U|^2 dk = \varepsilon$ then there exists $R_0 > 0$ such that $\sup_{\bar{k} \in B_{R_0}(k_0)} \sup_{0 < R \leq R_0} R^{2-d} \int_{B_R(\bar{k})} |\nabla U|^2 dk \leq 2\varepsilon$, *i.e.* at sufficiently small scales the scaled energy is locally uniformly bounded by its limit at any point.

The second ingredient is a compactness theorem for the scaled maps $U_R(k) = U(k_0 + Rk)$ which is similar to the compactness theorem for minimizing harmonic maps (see [SU1] and [Si], Chapter 2).

Proposition 4.8. *Let $d \geq 3$ and $U \in W^{1,2}(\mathbb{T}_d^*; \mathcal{U}(m))$ be a minimizer of the localization functional* (3.5)*. If we define $U_R(k) = U(k_0 + Rk)$, $R > 0$, then up to subsequences $U_R \to U_0$ strongly in $W^{1,2}_{\mathrm{loc}}(\mathbb{R}^d; \mathcal{U}(m))$. In addition U_0 is a locally minimizing harmonic map and it is degree-zero homogeneous.*

To prove the previous result we need the following two auxiliary lemmas. The first is a simple consequence of local minimality. The second is a nonlinear interpolation lemma due to Luckhaus which we state in our specific context (for the general case see e.g. [LW1], Lemma 2.2.9; see also [Si], Chapter 2 for a proof).

Lemma 4.9. *Suppose U and U_R as in Proposition 4.8. Let $\rho \in (0,1)$ and let $\{v_R\} \subset W^{1,2}(B_\rho; \mathcal{U}(m))$ a bounded sequence such that $U_R = v_R$ on ∂B_ρ for each $R > 0$. Then*

$$\liminf_{R \to 0} \int_{B_\rho} |\nabla U_R|^2 \leq \liminf_{R \to 0} \int_{B_\rho} |\nabla v_R|^2 .$$

Proof. Define $\tilde{v}_R(k) = v_R(R^{-1}(k-k_0))$ so that $\tilde{v}_R \in W^{1,2}(B_{\rho R}(k_0);\mathcal{U}(m))$. Since $\tilde{v}_R = U$ on $\partial B_{\rho R}(k_0)$ we can extend them as U to the whole $\mathbb{T}_d^*$. The assumption on v_R and Proposition 4.6 clearly imply $\int_{B_{\rho R}(k_0)} |\nabla U|^2 + |\nabla \tilde{v}_R|^2 = \mathcal{O}(R^{d-2})$ as $R \to 0$, hence formula (3.5) and simple calculations using Cauchy-Schwartz inequality give

$$\tilde{F}_{MV}(\tilde{v}_R;\chi) - \tilde{F}_{MV}(U;\chi) = \int_{B_{\rho R}(k_0)} |\nabla \tilde{v}_R|^2 - \int_{B_{\rho R}(k_0)} |\nabla U|^2 + \mathcal{O}(R^{d-1})\,, \tag{4.16}$$

because $\tilde{v}_R$ and U coincide outside $B_{\rho R}(k_0)$. Since U is a minimizer of $\tilde{F}_{MV}$ the right hand side of (4.16) is nonnegative, hence scaling back and taking the definition of U_R and $\tilde{v}_R$ into account the conclusion follows as $R \to 0$. □

Lemma 4.10 (Luckhaus). *Let $d \geq 3$, $m \geq 2$ and let $u, v \in W^{1,2}(S^{d-1};\mathcal{U}(m))$. Then, for each $\lambda \in (0,1)$ there is $w \in W^{1,2}(S^{d-1} \times (1-\lambda,1); M_m(\mathbb{C}))$ such that $w|_{S^{d-1}\times\{1\}} = u$, $w|_{S^{d-1}\times\{1-\lambda\}} = v$,*

$$\int_{S^{d-1}\times(1-\lambda,1)} |\nabla w|^2 \leq C\lambda \int_{S^{d-1}} \left(|\nabla_T u|^2 + |\nabla_T v|^2\right) + C\lambda^{-1} \int_{S^{d-1}} |u-v|^2 \tag{4.17}$$

and

$$\operatorname{dist}^2(w(k),\mathcal{U}(m)) \leq C\lambda^{1-d} \left(\int_{S^{d-1}} \left(|\nabla_T u|^2 + |\nabla_T v|^2\right)\right)^{\frac{1}{2}} \left(\int_{S^{d-1}} |u-v|^2\right)^{\frac{1}{2}} +$$

$$+ C\lambda^{-d} \int_{S^{d-1}} |u-v|^2 \tag{4.18}$$

for a.e. $k \in S^{d-1} \times (1-\lambda,1)$. Here ∇_T is the gradient on S^{d-1}.

Proof of Proposition 4.8. We essentially follow the proof of [LW1], Lemma 2.2.13, with minor modifications. By Proposition 4.6, up to subsequences we may assume $U_R \rightharpoonup U_0$ in $W^{1,2}(B_1;\mathcal{U}(m))$ where U_0 is a degree-zero homogeneous map. Thus, it is enough to show strong convergence and minimality in some ball $B_\rho \subset B_1$ to get the same properties on any $B_\rho \subset \mathbb{R}^d$ for any $\rho > 0$, by scale invariance of U_0 and the existence of the full limit of $R^{2-d}\int_{B_R} |\nabla U|^2$ as $R \to 0$.

Let $B_1 \subset \mathbb{R}^d$ and $\delta \in (0,1)$ a fixed number and let $\bar{w} \in W^{1,2}(B_1;\mathcal{U}(m))$ such that $\bar{w} \equiv U_0$ a.e. on $B_1 \setminus B_{1-\delta}$. By Fatou's lemma and Fubini's theorem, there is $\rho \in (1-\delta,1)$ such that

$$\lim_{R\to 0} \int_{\partial B_\rho} |U_R - U_0|^2 dH^{d-1} = 0\,, \quad \int_{\partial B_\rho} \left(|\nabla U_R|^2 + |\nabla U_0|^2\right) dH^{d-1} \leq C < \infty\,.$$

Applying Lemma 4.10 to $\lambda = \lambda_R < \delta$, $u = U_R(\rho\,\cdot)$ and $v = \bar{w}(\rho\,\cdot) \equiv U_0(\rho\,\cdot)$ for a decreasing sequence of numbers $\lambda_R \to 0$, we conclude that there exists a sequence of maps $w_R \in W^{1,2}(B_\rho; M_m(\mathbb{C}))$ such that if we chose e.g. $\lambda_R = \left(\int_{\partial B_\rho} |U_R - U_0|^2 dH^{d-1}\right)^{1/2d} < \delta$, then we have

$$w_R(k) = \begin{cases} \bar{w}\left(\frac{k}{1-\lambda_R}\right)\,, & |k| \leq \rho(1-\lambda_R)\,, \\ U_R(k)\,, & |k| = \rho\,, \end{cases}$$

(4.19)
$$\int_{B_\rho \setminus B_{\rho(1-\lambda_R)}} |\nabla w_R|^2 \leq C \left[\lambda_R \int_{\partial B_\rho} \left(|\nabla_T U_R|^2 + |\nabla_T U_0|^2 \right) + \lambda_R^{-1} \int_{\partial B_\rho} |U_R - U_0|^2 \right] \overset{R \to 0}{\longrightarrow} 0\,,$$
and $\operatorname{dist}(w_R, \mathcal{U}(m)) \to 0$ uniformly on $B_\rho \setminus B_{\rho(1-\lambda_R)}$ as $R \to 0$. Define comparison maps $\{v_R\} \subset W^{1,2}(B_\rho; \mathcal{U}(m))$ by

$$v_R(k) = \begin{cases} \bar{w}\left(\frac{k}{1-\lambda_R}\right), & |k| \leq \rho(1-\lambda_R)\,, \\ \Pi(w_R(k))\,, & \rho(1-\lambda_R) \leq |k| \leq \rho\,, \end{cases} \tag{4.20}$$

where $\Pi : \mathcal{O} \to \mathcal{U}(m)$ is the nearest point projection. Then, by minimality of U_R, Lemma 4.9 and (4.19)-(4.20) we obtain

$$\begin{aligned} \int_{B_\rho} |\nabla U_0|^2 &\leq \liminf_{R \to 0} \int_{B_\rho} |\nabla U_R|^2 \leq \liminf_{R \to 0} \int_{B_\rho} |\nabla v_R|^2 \\ &= \lim_{R \to 0} \left[\int_{B_{\rho(1-\lambda_R)}} \left| \nabla \bar{w} \left(\frac{\cdot}{1-\lambda_R} \right) \right|^2 + \int_{B_\rho \setminus B_{\rho(1-\lambda_R)}} |\nabla (\Pi \circ w_R)|^2 \right] \\ &\leq \lim_{R \to 0} \left[(1-\lambda_R)^{d-2} \int_{B_\rho} |\nabla \bar{w}|^2 + C \operatorname{Lip}(\Pi)^2 \int_{B_\rho \setminus B_{\rho(1-\lambda_R)}} |\nabla w_R|^2 \right] = \int_{B_\rho} |\nabla \bar{w}|^2 \,. \end{aligned}$$

Since $\bar{w}$ is arbitrary, the previous inequality implies both minimality of U_0 and strong convergence $U_R \to U_0$ in $W^{1,2}(B_\rho; \mathcal{U}(m))$ as $R \to 0$ and concludes the proof. □

The final ingredient is the following small-energy regularity result in the spirit of the fundamental $\varepsilon-$regularity theorem for harmonic maps proved in [SU1]. The result is similar to [Mos, Proposition 4.1] but the stationarity condition as well as the argument of the proof there (the so-called "moving-frame" trick) are different. Here we modify the elementary approach to regularity of [CWY] for harmonic maps into spheres, by rewriting the right hand side of (3.14)-(4.3) in a suitable way and applying a standard estimate for the Laplace equation. Then, an iteration argument gives the decay of the BMO norm at small scales, whence continuity follows from the equivalence of Morrey-Campanato spaces and Hölder spaces in a suitable range of parameters.

Proposition 4.11. *Let $d \geq 3$ and $U \in W^{1,2}(\mathbb{T}_d^*; \mathcal{U}(m))$ be a weak solution to the equations (3.14). Then there exist $\varepsilon > 0$ and $\beta > 0$, both independent of U and $k_0 \in \mathbb{T}_d^*$, such that if*

$$\sup_{\bar{k} \in B_{R_0}(k_0)} \sup_{0 < R \leq R_0} R^{2-d} \int_{B_R(\bar{k})} |\nabla U|^2 dk \leq \varepsilon$$

for some $R_0 > 0$, then $U \in C^{0,\beta}(B_{R_0/2}(k_0); \mathcal{U}(m))$.

Before going into the proof we quote two auxiliary results. First, recall that by definition for an open set $\Omega \subset \mathbb{R}^d$ a function $u \in L^1_{\mathrm{loc}}(\Omega)$ is in $BMO(\Omega)$ if

$$\|u\|_{BMO(\Omega)} = \sup_D ⨍_D |u - u_D| < \infty\,, \tag{4.21}$$

where $u_D = ⨍_D u$ is the average of u over D and the supremum is taken over all balls $D \subset \Omega$. The first fact we need is a classical result of John and Nirenberg (see [St], Chapter 4).

Lemma 4.12. *For any $1 < p < \infty$, there exists a constant $C_p > 0$ (which depends only on p and d) such that if $u \in BMO(\Omega)$ then*

$$\|u\|_{BMO(\Omega)} \leq \sup_D \left(\fint_D |u - u_D|^p \right)^{1/p} \leq C_p \|u\|_{BMO(\Omega)} < \infty \,, \tag{4.22}$$

where the supremum is taken over all balls $D \subset \Omega \subset \mathbb{R}^d$.

The second auxiliary result is a standard regularity property for solutions to the Laplace equation.

Lemma 4.13. *Let $d \geq 3$ and $B_{\bar{R}} \subset \mathbb{R}^d$ be an open ball of radius $\bar{R} > 0$. Let $q \in (\frac{d}{d-1}, 2)$, $s = \frac{qd}{q+d}$. There exist $C > 0$ depending only on q such that if $F \in L^2(B_{\bar{R}}; \mathbb{R}^d)$, $g \in L^2(B_{\bar{R}})$ and $u \in W_0^{1,2}(B_{\bar{R}})$ is a weak solution to $\Delta u = \operatorname{div} F + g$, then*

$$\|\nabla u\|_{L^q(B_{\bar{R}})} \leq C \left(\|F\|_{L^q(B_{\bar{R}})} + \|g\|_{L^s(B_{\bar{R}})} \right) . \tag{4.23}$$

Proof of Proposition 4.11. First note that if U satisfies the condition

$$\sup_{\bar{k} \in B_{R_0}(k_0)} \sup_{0 < R \leq R_0} R^{2-d} \int_{B_R(\bar{k})} |\nabla U|^2 dk \leq \varepsilon \quad \text{for some } R_0 > 0 \,,$$

then on $B_{R_0} = B_{R_0}(k_0)$, by Cauchy-Schwartz and Poincaré inequality we have

(4.24)
$$\|U\|_{BMO(B_{R_0})} \leq \sup_{D_R \subset B_{R_0}} \left(\fint_{D_R} |U - \fint_{D_R} U|^2 \right)^{1/2} \leq C \sup_{D_R \subset B_{R_0}} \left(R^2 \fint_{D_R} |\nabla U|^2 \right)^{1/2} \leq C \varepsilon^{1/2} \,.$$

Now, we aim to show that, for ε sufficiently small, there is a quantitative decay of the BMO norm of U at smaller and smaller scales.

Up to translation we may assume $k_0 = 0$. Let $\sigma \in (0, \frac{1}{8}]$ a fixed number to be specified later. For each $\widehat{k} \in B_{R_0/2}$ and $t \in (0, R_0/2]$, let $D_t = D_t(\widehat{k}) \subset B_{R_0}$ be an open ball of radius t, and for each $\bar{k} \in D_{\sigma t} = D_{\sigma t}(\widehat{k})$ let $R \in (0, t)$ be such that $B_{\sigma R}(\bar{k}) \subset D_{\sigma t}$. Clearly, $B_{R(\bar{k})} \subset D_t \subset B_{R_0}$, so that if $\bar{R} \in (R/2, R)$ we still have the bound $\bar{R}^{2-d} \int_{B_{\bar{R}}(\bar{k})} |\nabla U|^2 dk \leq \varepsilon$.

On the other hand, given a constant matrix $T_0 \in M_m(\mathbb{C})$ with $|T_0| \leq \sqrt{m}$, e.g. $T_0 = \fint_{B_R(\bar{k})} U$, we may choose $\bar{R} \in (R/2, R)$ so that

$$\int_{\partial B_{\bar{R}}(\bar{k})} |U - T_0| \leq 8 \int_{B_R(\bar{k})} |U - T_0| \,. \tag{4.25}$$

Since $U|_{\partial B_{\bar{R}}} \in W^{1/2,2}(\partial B_{\bar{R}}; \mathcal{U}(m))$ there exists a harmonic extension $h \in W^{1,2}(B_{\bar{R}}; M_m(\mathbb{C})$ so that h=$U|_{\partial B_{\bar{R}}}$ on $\partial B_{\bar{R}}$ and $h \in C^\infty$ in the interior. Moreover, mean value formula, Jensen's inequality and (4.25) easily give

$$|\nabla h(k)|^p \leq C_p \bar{R}^{-p} \fint_{B_R(\bar{k})} |U - T_0|^p \tag{4.26}$$

for any $p \in (1, \infty)$ and any $k \in B_{\frac{1}{4}\bar{R}}(\bar{k})$.

On the other hand, as in the two dimensional case, since $U \in W^{1,2}(\mathbb{T}^*_d;\mathcal{U}(m))$ is a weak solution to (3.14), we have

$$\Delta U = \sum_{j=1}^{d} \frac{\partial U}{\partial k_j} U^{-1} \frac{\partial U}{\partial k_j} + f\,, \tag{4.27}$$

for some L^2 function f such that $U^{-1}f \in L^2(\mathbb{T}^*_d;\mathfrak{u}(m))$. As in Proposition 4.3, if we set $B^j = \frac{1}{2}\left(U^*\frac{\partial U}{\partial k_j} - \frac{\partial U^*}{\partial k_j}U\right)$ then $B^j \in L^2(\mathbb{T}^*_d;\mathfrak{u}(m))$ for $j = 1,\dots,d$ and $U - h \in W^{1,2}_0(B_{\bar{R}}(\bar{k}); M_m(\mathbb{C}))$ is a weak solution to

$$\begin{aligned}\Delta(U-h) &= \sum_{j=1}^{d} \frac{\partial U}{\partial k_j} B^j + f = \sum_{j=1}^{d} \frac{\partial}{\partial k_j}\left((U-T_0)B^j\right) + f - (U-T_0)\sum_{j=1}^{d} \frac{\partial B_j}{\partial k_j} = \\ &= \sum_{j=1}^{d} \frac{\partial}{\partial k_j}\left((U-T_0)B^j\right) + f - (U-T_0)\frac{1}{2}(U^*f - fU^*) = \operatorname{div} F + g\,.\end{aligned} \tag{4.28}$$

Since $|B(k)| \le C|\nabla U(k)|$ and $|g(k)| \le C|f(k)| \le C(1+|\nabla U(k)|)$, for the right hand side of (4.28) we have the straightforward estimates

$$\|F\|_{L^q(B_{\bar{R}}(\bar{k}))} \le \|\nabla U\|_{L^2(B_{\bar{R}}(\bar{k}))}\|U-T_0\|_{L^{\frac{2q}{2-q}}(B_{\bar{R}}(\bar{k}))} \le \|U-T_0\|_{L^{\frac{2q}{2-q}}(B_{\bar{R}}(\bar{k}))}\sqrt{\varepsilon}\bar{R}^{\frac{d-2}{2}}\,. \tag{4.29}$$

and

$$\|g\|_{L^s(B_{\bar{R}}(\bar{k}))} \le C\bar{R}^{\frac{d}{s}} + C\|\nabla U\|_{L^s(B_{\bar{R}}(\bar{k}))} \le C\bar{R}^{\frac{d-2}{2}}\left(\bar{R}^{2+d\left(\frac{1}{q}-\frac{1}{2}\right)} + \sqrt{\varepsilon}\bar{R}^{d\frac{2-s}{2}}\right)\,. \tag{4.30}$$

Applying Lemma 4.13 to (4.28) and taking (4.29) and (4.30) into account we obtain

$$\int_{B_{\bar{R}}(\bar{k})} |\nabla(U-h)|^q \le C_q\varepsilon^{\frac{q}{2}}\bar{R}^{q\frac{d-2}{2}}\|U-T_0\|^q_{L^{\frac{2q}{2-q}}(B_{\bar{R}}(\bar{k}))} + C_q\bar{R}^{q\frac{d-2}{2}}\left(\bar{R}^{2q+d\frac{2-q}{2}} + \varepsilon^{\frac{q}{2}}\bar{R}^{qd\frac{2-s}{2}}\right)\,, \tag{4.31}$$

i.e.

$$\fint_{B_{\bar{R}}(\bar{k})} |\nabla(U-h)|^q \le C_q\bar{R}^{-q}\left[\varepsilon^{\frac{q}{2}}\left(\fint_{B_{\bar{R}}(\bar{k})} |U-T_0|^{\frac{2q}{2-q}}\right)^{\frac{2-q}{2}} + C_q\bar{R}^{2q} + C_q\varepsilon^{\frac{q}{2}}\bar{R}^{qd\frac{2-s}{2}+q\frac{d}{2}-d}\right]\,. \tag{4.32}$$

Now we choose $p = q^* = \frac{dq}{d-q} > q$ and $\underline{R} = \sigma R < \bar{R} < R$. Using Sobolev inequality, (4.32) and (4.26) we estimate

$$\begin{aligned}\fint_{B_{\sigma R}(\bar{k})} |U - h(\bar{k})|^p &\le \frac{C}{\underline{R}^d}\int_{B_{\bar{R}}(\bar{k})} |U-h|^p + \frac{C}{\underline{R}^d}\int_{B_{\underline{R}}(\bar{k})} |h-h(\bar{k})|^p \\ &\le C\frac{\bar{R}^{d+p}}{\underline{R}^d}\left(\fint_{B_{\bar{R}}(\bar{k})} |\nabla(U-h)|^q\right)^{\frac{p}{q}} + C\underline{R}^p \sup_{B_{\bar{R}/4}} |\nabla h|^p\end{aligned}$$

$$\le C\sigma^{-d}\left(\varepsilon^{\frac{q}{2}}\left(\fint_{B_{\bar R}(\bar k)}|U-T_0|^{\frac{2q}{2-q}}\right)^{\frac{2-q}{2}}+C_q\bar R^{2q}+C_q\varepsilon^{\frac{q}{2}}\bar R^{qd\frac{2-s}{2}+q\frac{d}{2}-d}\right)^{\frac{p}{q}}+C\sigma^p\fint_{B_R(\bar k)}|U-T_0|^p$$

$$\le C\sigma^{-d}\left(\varepsilon^{\frac{p}{2}}\left(\fint_{B_R(\bar k)}|U-T_0|^{\frac{2q}{2-q}}\right)^{p\frac{2-q}{2q}}+R^{2p}+\varepsilon^{\frac{p}{2}}R^{pd\frac{2-s}{2}+p\frac{d}{2}-p-d}\right)+C\sigma^p\fint_{B_R(\bar k)}|U-T_0|^p$$

Since $B_R(\bar k)\subset D_t$, if we choose $T_0=\fint_{B_R(\bar k)}U$ the John-Nirenberg inequality (4.22) yields

(4.33)

$$\left(\fint_{B_{\sigma R}(\bar k)}|U-h(\bar k)|^p\right)^{1/p}\le\left(\sigma^{-d/p}\varepsilon^{1/2}+\sigma\right)C_q\|U\|_{BMO(D_t)}+C_q\sigma^{-d/p}\left(t^{2p}+\varepsilon^{\frac{p}{2}}t^{pd\frac{2-s}{2}+p\frac{d}{2}-p-d}\right).$$

On the other hand, by Hölder inequality and (4.33) we get

$$\fint_{B_{\sigma R}(\bar k)}|U-\fint_{B_{\sigma R}(\bar k)}U|\le\left(\fint_{B_{\sigma R}(\bar k)}|U-h(\bar k)|^2\right)^{1/2}\le\left(\fint_{B_{\sigma R}(\bar k)}|U-h(\bar k)|^p\right)^{1/p}$$
$$\le\left(\sigma^{-d/p}\varepsilon^{1/2}+\sigma\right)C_q\|U\|_{BMO(D_t)}+C_q\sigma^{-d/p}\left(t^{2p}+\varepsilon^{\frac{p}{2}}t^{pd\frac{2-s}{2}+p\frac{d}{2}-p-d}\right),\tag{4.34}$$

hence, taking the supremum over $B_{\sigma R}(\bar k)\subset D_{\sigma t}$ we obtain

(4.35)

$$\|U\|_{BMO(D_{\sigma t})}\le\left(\sigma^{-d/p}\varepsilon^{1/2}+\sigma\right)C_q\|U\|_{BMO(D_t)}+C_q\sigma^{-d/p}\left(t^{2p}+\varepsilon^{\frac{p}{2}}t^{pd\frac{2-s}{2}+p\frac{d}{2}-p-d}\right).$$

Since $p=p(q)$, $s=s(q)$, the exponent $\alpha:=pd\frac{2-s}{2}+p\frac{d}{2}-p-d\to 1$ as $q\searrow\frac{d}{d-1}$ so we can fix q small such that $\alpha\in(0,2)$. If we choose $\sigma\in(0,\frac18]$ and $\varepsilon>0$ so small that $C_q(\sigma^{-d/p}\varepsilon^{1/2}+\sigma)<\frac12$ then

$$\|U\|_{BMO(D_{\sigma t})}\le\frac12\|U\|_{BMO(D_t)}+Ct^{\alpha}\,,\qquad\forall t\in(0,R_0/2]\,,\tag{4.36}$$

where $C>0$ and $\alpha\in(0,2)$ are independent of U, $\widehat k$ and t. Thus, from (4.36) an elementary iteration argument on $v(t)=\|U\|_{BMO(D_t)}$ and the John-Nirenberg inequality (4.22) give

$$\fint_{D_t(\widehat k)}|U-\fint_{D_t(\widehat k)}U|^2\le Ct^{2\beta}\,,\qquad\forall t\in(0,R_0/2]\,,\quad\forall\widehat k\in B_{R_0/2}\,,\tag{4.37}$$

for some $\beta=\beta(\alpha)>0$. Finally, from [Ca] we conclude that $U\in C^{0,\beta}(B_{R_0/2};\mathcal U(m))$ and the proof is complete. □

Combining the previous propositions and the Liouville type theorem proved in the Appendix we have the main result of this section.

Theorem 4.14. *Let $d=3$ and $U\in W^{1,2}(\mathbb T^*_d;\mathcal U(m))$ be a minimizer of the localization functional* (3.5). *If $2\le m\le 3$ then $U\in C^0(\mathbb T^*_d;\mathcal U(m))$.*

Proof. Fix $k_0\in\mathbb T^*_3$ and for each $R=R_n\searrow 0$ we define $U_R(k)=U(k_0+Rk)$. According to Proposition 4.6 such a sequence is bounded in $W^{1,2}_{\rm loc}(\mathbb R^3;\mathcal U(m))$ and, up to subsequences, it converges weakly to a degree-zero homogeneous map $U_0\in W^{1,2}_{\rm loc}(\mathbb R^3;\mathcal U(m))$. According to Proposition 4.8, such convergence is strong and the limiting map U_0 is a degree-zero homogeneous local minimizer of the Dirichlet integral in $W^{1,2}_{\rm loc}(\mathbb R^3;\mathcal U(m))$. According to Corollary

A.10, when $2 \leq m \leq 3$ we have $U_0(k) \equiv const$, therefore $\frac{1}{R_n} \int_{B_{R_n}(k_0)} |\nabla U|^2 = \int_{B_1} |\nabla U_{R_n}|^2 \to 0$ as $n \to \infty$, hence it can be made arbitrarily small at sufficiently small scale. Thus, in view of Proposition 4.11 continuity around k_0 follows, and $U \in C^0(\mathbb{T}^*_3; \mathcal{U}(m))$ since k_0 was arbitrary. □

5. Analytic regularity

In this section we first prove analytic regularity for continuous weak solutions to the Euler Lagrange equations (3.14), whenever χ is a real-analytic Bloch frame (*i.e.* $A_j \in C^\omega(\mathbb{T}^*_d, \mathfrak{u}(m))$). Then, combining this property with the continuity results for the minimizers of the localization functional (3.5), we prove analyticity for any minimizer of the functionals (3.4) and (3.5).

We start with the following auxiliary result.

Proposition 5.1. *Assume $d \geq 2$. Let χ be a real-analytic Bloch frame and $U \in W^{1,2}(\mathbb{T}^*_d; \mathcal{U}(m))$ be a weak solution to equation* (3.14). *If $U \in C^0(\mathbb{T}^*_d; \mathcal{U}(m))$ then $U \in W^{1,4}(\mathbb{T}^*_d; \mathcal{U}(m))$ and $U \in W^{2,2}(\mathbb{T}^*_d; \mathcal{U}(m))$.*

Proof. We rewrite the system (3.14) in the form

$$\Delta U = \mathcal{F}(A(k), U, \nabla U) = F(k, U, \nabla U)\,, \tag{5.1}$$

where $\mathcal{F} : (M_m(\mathbb{C}))^d \times M_m(\mathbb{C}) \times (M_m(\mathbb{C}))^d \to M_m(\mathbb{C})$ is a real-analytic (polynomial) map and the matrices $A(k) = (A_1(k), \ldots, A_d(k))$, *i.e.* the entries of the Berry connection given in (3.6), are real-analytic on the torus $\mathbb{T}^*_d$. It is easy to see that, since A is smooth and U takes values into $\mathcal{U}(m)$, by construction the function $F(k, s, p)$ on the range of U satisfies the structural assumptions

$$|F(k,s,p)| + |\nabla_s F(k,s,p)| \leq c_0(1+|p|^2)\,, \qquad |\nabla_k F(k,s,p)| + |\nabla_p F(k,s,p)| \leq c_1(1+|p|) \tag{5.2}$$

on $\mathbb{T}^*_d \times \mathcal{U}(m) \times (M_m(\mathbb{C}))^d$.

As a consequence of [Jo], Lemma 8.5.1 and Lemma 8.5.3, any continuous weak solution U of (5.1) is locally in $W^{2,2} \cap W^{1,4}$ and the conclusion follows taking a finite cover of the torus. □

Combining the previous result with the standard regularity theory for linear elliptic equations and the fundamental analyticity results for nonlinear elliptic systems (see *e.g.* [Mor], Chapter VI), we obtain full regularity. The proof is standard, so we just sketch it for the reader's convenience.

Proposition 5.2. *Let $d = 2$ or $d = 3$ and let $U \in W^{1,2}(\mathbb{T}^*_d; \mathcal{U}(m))$ be a weak solution to equation* (3.14). *If χ is real-analytic and $U \in C^0(\mathbb{T}^*_d; \mathcal{U}(m))$, then U is real-analytic.*

Proof. According to Proposition 5.1 we know that $U \in W^{1,4}(\mathbb{T}^*_d; \mathcal{U}(m))$ and $U \in W^{2,2}(\mathbb{T}^*_d; \mathcal{U}(m))$. If $d = 2$ then Sobolev embedding yields $\nabla U \in L^p$ for any $p < \infty$. Similarly, in case $d = 3$ we have $\nabla U \in L^6$, hence (5.2) implies $G(k, U, \nabla U) \in L^3$. Thus, linear elliptic regularity for (5.1) gives $U \in W^{2,3}$ and in turn $\nabla U \in L^p$ for any $p < \infty$ again by Sobolev embedding (note that the same property holds for any $d \geq 4$, compare [Jo, Lemma 8.5.4]). Clearly, if $\nabla U \in L^p$ for any $p < \infty$ the same is true for $G(k, U, \nabla U)$ because of (5.2), hence linear elliptic regularity for (5.1) gives $U \in W^{2,p}$ for any $p < \infty$, which in turn yields $U \in C^{1,\alpha}$ for any $\alpha \in (0, 1)$ by Sobolev-Morrey embedding. Going back to (3.14) a standard bootstrap argument in the Hölder spaces $C^{l,\alpha}$, $l \geq 1$, yields by induction $U \in C^{l,\alpha} \Rightarrow \Delta U \in C^{l-1,\alpha} \Rightarrow U \in C^{l+1,\alpha}$, so that $U \in C^\infty(\mathbb{T}^*_d;\mathcal{U}(m))$. Finally, since the coefficients A_j in (3.14) are analytic, by the results in [Mor], Chapter VI, any smooth solution is real-analytic. $\square$

The main result of the section is the following.

Theorem 5.3. *Let $1 \le d \le 2$ and $m \ge 1$, or $d = 3$ and $1 \le m \le 3$, or $d \ge 4$ and $m = 1$. Let χ be a real-analytic Bloch frame and $\tilde{F}_{MV}(\cdot)$ and $\tilde{F}_{MV}(\cdot\,;\chi)$ the functionals defined by (3.4) and (3.5) respectively. Then:*

(i) *any minimizer $U \in W^{1,2}(\mathbb{T}^*_d;\mathcal{U}(m))$ of $\tilde{F}_{MV}(\cdot\,;\chi)$ is real-analytic;*
(ii) *any minimizer $\varphi = \{\varphi_1, \dots, \varphi_m\} \subset \tilde{\mathcal{W}}$ of $\tilde{F}_{MV}(\cdot)$ is a real-analytic map from $\mathbb{R}^d$ to $(\mathcal{H}_{\mathrm{f}})^m$.*

Proof. (i) Since any minimizer U is a weak solution to (3.14) and χ is real-analytic, the conclusion follows from Proposition 4.1 if $d = 1$ or $m = 1$, and from Corollary 4.4, Theorem 4.14 and Proposition 5.2 in the other cases.

(ii) Let $w = \tilde{\mathcal{U}}_{\mathrm{BF}}^{-1}\varphi$ and $\varphi = \chi \cdot U$. Then $F_{MV}(w) = \tilde{F}_{MV}(\varphi) = \tilde{F}_{MV}(U;\chi)$, U is a minimizer of the latter functional in view of (3.7), and the conclusion follows from part (i) above. $\square$

6. Exponential localization of maximally localized Wannier functions

The main result of the paper is the following, and provides an affirmative answer to problems (MV_1) and (MV_2).

Theorem 6.1. *Let σ_* be a family of m Bloch bands for the operator (1.1) satisfying the gap condition (2.9), and let $\{P_*(k)\}_{k\in\mathbb{R}^d}$ be the corresponding family of spectral projectors. Assume $d \le 2$ and $m \ge 1$, or $d \ge 1$ and $m = 1$, or $d = 3$ and $1 \le m \le 3$. Then there exist composite Wannier functions $\{w_1, \dots, w_m\} \subset \mathcal{W}$ which minimize the localization functional* (3.2) *under the constraint that the corresponding quasi-Bloch functions are an orthonormal basis for* Ran $P_*(k)$ *for each $k \in Y^*$. In addition, for any system of maximally localized composite Wannier function $w = \{w_1, \dots, w_m\}$ there exists $\beta > 0$ such that $e^{\beta|x|}w_a$ is in $L^2(\mathbb{R}^d)$ for every $a \in \{1, \dots, m\}$, 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 appearing in (2.10).

Proof. In view of Theorem 2.9, there exists a Bloch frame χ which is real-analytic. Therefore, problem (MV_1) is equivalent to showing that the r.h.s. of (3.7) is attained, which is proved in Theorem 3.4.

Let $w = \{w_1, \dots w_m\} \subset \mathcal{W}$ be any minimizer of F_{MV}. Then $\varphi_a := \tilde{\mathcal{U}}_{\mathrm{BF}} w_a$ defines a minimizer $\{\varphi_1, \dots, \varphi_m\} \subset \tilde{\mathcal{W}}$ of $\tilde{F}_{MV}$ among the Bloch frames. With respect to the frame χ, one has $\varphi = \chi \cdot U$, where $U \in W^{1,2}(\mathbb{T}^*_d;\mathcal{U}(m))$ is given by $U_{b,a}(k) = \langle \chi_b(k)\,,\,\varphi_a(k)\rangle$. Clearly, U is a minimizer of $\tilde{F}_{MV}(\cdot\,;\chi)$. By Theorem 5.3, $U \in W^{1,2}(\mathbb{T}^*_d;\mathcal{U}(m))$ is actually real-analytic.

The function U defines a real-analytic Γ^*-periodic function $\tilde{U} : \mathbb{R}^d \to \mathcal{U}(m)$. By unique continuation, $\tilde{U}$ extends to a holomorphic function $\tilde{U}^{\mathbb{C}}$ from Ω_{β_1} to $\mathrm{GL}(m, \mathbb{C})$, which is Γ^*-periodic in the real part of its argument. Analogously, arguing as in the proof of Proposition

2.1, χ admits a holomorphic extension $\chi^{\mathbb{C}} \in \mathcal{H}^{\mathbb{C}}_{\tau,\beta_2}$ for some $\beta_2 > 0$. Therefore $\varphi = \chi \cdot U$ is a real-analytic Bloch frame which admits a holomorphic extension $\varphi^{\mathbb{C}} = \chi^{\mathbb{C}} \cdot \tilde{U}^{\mathbb{C}}$, which is in $\mathcal{H}^{\mathbb{C}}_{\tau,\beta_0}$ for $\beta_0 = \min\{\beta_1, \beta_2, \alpha\}$. Moreover, for any $\beta < \beta_0$ there exists C such that

$$\int_{Y*} \|\varphi^{\mathbb{C}}(k + ih)\|^2 \, dk < C$$

for every h such that $|h_j| \leq \beta$ for $j \in \{1, \dots, d\}$. By Proposition 2.3 one has that $w_a := \tilde{\mathcal{U}}^{-1}_{\mathrm{BF}} \, \varphi_a$ satisfies

$$\int e^{2\beta|x|} \, |w_a(x)|^2 \, dx < +\infty.$$

$\square$

Appendix A. Harmonic maps into $\mathcal{U}(m)$

We consider, for $\Omega' = \mathbb{R}^3 \setminus \{0\}$ and $U \in W^{1,2}_{\mathrm{loc}}(\Omega'; \mathcal{U}(m))$ with $m \geq 2$, the energy functional

$$E(U; \Omega) = \int_\Omega \frac{1}{2} \sum_{j=1}^{3} \operatorname{tr}\left(\frac{\partial U^*}{\partial k_j} \frac{\partial U}{\partial k_j} \right) dk\,, \qquad \Omega \subset\subset \Omega'. \tag{A.1}$$

We assume that U is a local minimizer of (A.1) in Ω', *i.e.* that $E(U; \Omega) \leq E(W; \Omega)$ for any $\Omega \subset\subset \Omega'$ and for any $W \in W^{1,2}_{\mathrm{loc}}(\Omega'; \mathcal{U}(m))$ such that $\mathrm{supp}(U - W) \subset\subset \Omega$. Clearly, if $\Psi \in C^\infty_0(\Omega; \mathfrak{u}(m))$ and $\varepsilon \in \mathbb{R}$, then $U_\varepsilon(k) = U(k) \exp \varepsilon \Psi(k)$ is an admissible variation of U, hence local minimality gives

$$\left.\frac{d}{d\varepsilon}\right|_{\varepsilon=0} E(U_\varepsilon; \Omega) = 0\,, \qquad \left.\frac{d^2}{d\varepsilon^2}\right|_{\varepsilon=0} E(U_\varepsilon; \Omega) \geq 0\,. \tag{A.2}$$

Since the tangential variation Ψ can be chosen arbitrarily, the first condition in (A.2) easily implies that U is a weakly harmonic map, *i.e.* U is a weak solution to

$$-\Delta U + \sum_{j=1}^{3} \frac{\partial U}{\partial k_j} U^{-1} \frac{\partial U}{\partial k_j} = 0\,. \tag{A.3}$$

We aim to prove that, when $m \geq 2$, any local minimizer $U \in W^{1,2}_{\mathrm{loc}}(\Omega'; \mathcal{U}(m))$ which is degree-zero homogeneous (a minimizing tangent map), *i.e.*

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

is constant. The argument we are going to use combines a stability inequality derived from (A.2) (see inequality (A.12) below) and a nontrivial quantization property for the energy of every harmonic map $\omega \in C^\infty(S^2; \mathcal{U}(m))$ [Va, Corollary 8].
Actually, in view of Lemma A.1 below, when $m = 2$ this constancy property is known and it follows from [SU2, Proposition 1], since $\mathcal{SU}(2) \equiv S^3(\sqrt{2})$. However, when the target is a sphere, the constants in the stability inequalities are uniformly bounded as the dimension of the sphere increases (see [SU2, formula $(*)$]), which will not be the case in the problem we are dealing with. Here we prove, by a different technique, the constancy property in the case $m \leq 3$. In our opinion, if (A.12) cannot be improved, then it seems difficult to prove the Liouville property for any $m \geq 4$ using the so-called Bochner method as in the sphere-valued case (see [SU2] and [LW2]; see also [Xin, Chapter 5] and references therein).

As far as our specific problem is concerned, we can assume that the target is indeed the special unitary group $\mathcal{SU}(m)$ in view of the following auxiliary result.

Lemma A.1. *Let $d = 3$ and $m \geq 2$. Let $U \in W^{1,2}_{\mathrm{loc}}(\Omega'; \mathcal{U}(m))$ be a degree-zero homogeneous weakly harmonic map. Then* $\det U \equiv \alpha \in \mathcal{U}(1)$ *and* $U \in W^{1,2}_{\mathrm{loc}}(\Omega'; \mathcal{SU}(m))$ *up to multiplication by a constant unitary matrix U_0. As a consequence,* $\mathrm{tr}(U^* \partial_j U) \equiv 0$ *for each* $1 \leq j \leq 3$.

Proof. Clearly, $\det U \in W^{1,2}_{\mathrm{loc}}(\Omega'; \mathcal{U}(1))$ and it is degree-zero homogeneous. According to [BZ], if B is the unit ball, there exists $g \in W^{1,2}(B)$ such that $\det U = \mathrm{e}^{ig}$ a.e. in B. By slicing, g is $W^{1,2}_{\mathrm{loc}}$ on a.e. ray from the origin, so it is continuous along a.e. ray. Since $\mathrm{e}^{ig} = \det U$ is constant along the rays, we conclude that g is also constant along the rays, *i.e.* g is degree-zero homogeneous.

Let us set $\hat{U}(k) = \mathrm{e}^{\frac{i}{m} g(k)}\,\mathbb{I}$ and $W(k) = \hat{U}(k)^* U(k)$. By construction $\det \hat{U} \equiv \det U$, so that $W = \hat{U}^* U \in W^{1,2}(B; \mathcal{SU}(m))$. Thus, in order to prove the lemma it is clearly enough to show that g (and in turn $\hat{U}$) is constant in B, because the conclusion follows in the whole $\mathbb{R}^3$ since U is degree-zero homogeneous. Notice that if $\eta \in C_0^\infty(B)$, $\varepsilon \in \mathbb{R}$ and $g_\varepsilon = g + \varepsilon\eta$ then (A.4)

$$E(\mathrm{e}^{\frac{i}{m} g_\varepsilon}\mathbb{I}\, W; B) = \int_B \frac{1}{2m}|\nabla g_\varepsilon|^2 + \int_B \frac{1}{2}\sum_{j=1}^{3} \mathrm{tr}\left(\frac{\partial W^*}{\partial k_j}\frac{\partial W}{\partial k_j}\right) dk = E(\mathrm{e}^{\frac{i}{m} g_\varepsilon}\mathbb{I}; B) + E(W; B)\,.$$

Since $U_\varepsilon = \mathrm{e}^{\frac{i}{m} g_\varepsilon}\mathbb{I}\, W$ is an admissible variation for U, differentiating (A.4) we readily see that the function g is weakly harmonic in B, hence g is continuous (real-analytic). Since g is also degree-zero homogeneous we conclude that g is constant in B as claimed. As a consequence, $\hat{U}$ is constant, $\det U$ is also constant (both in B and in $\mathbb{R}^3$, both functions being degree-zero homogeneous) and $U \in W^{1,2}_{\mathrm{loc}}(\Omega'; \mathcal{SU}(m))$ up to multiplying by a constant unitary matrix $U_0 = \hat{U}^*$. Finally, since $U^*\partial_j U \in \mathfrak{su}(m)$ we also have $\mathrm{tr}\,(U^*\partial_j U) \equiv 0$ for each $1 \le j \le 3$. □

A.1. **The stability inequality.** Throughout this section we assume that U is a smooth harmonic map and we denote by V the variational vector field, *i.e.* $V(k) = \frac{d}{d\varepsilon}\big|_{\varepsilon=0} U_\varepsilon(k) = U_\varepsilon(k)\Psi(k)$ associated to the deformation $U_\varepsilon(k) = U(k)\exp^{\varepsilon\Psi(k)}$. We regard $\mathcal{SU}(m) \subset M_m(\mathbb{C})$ as a Riemannian manifold with the metric induced by the embedding in $M_m(\mathbb{C})$, the latter being equipped with the Hilbert-Schmidt inner product(2) $\langle A\,,\,B\rangle = \mathrm{Re}\,\mathrm{tr}(A^*B)$. The second variation formula for the energy [LW1, Chapter 1] yields

$$\left.\frac{d^2}{d\varepsilon^2}\right|_{\varepsilon=0} E(U_\varepsilon; \Omega) = \sum_j \int_\Omega \|\widetilde{\nabla}_{e_j} V\|^2 - R(dU(e_j), V, dU(e_j), V) \tag{A.5}$$

where $\{e_j\}$ is an orthonormal basis of $\mathbb{R}^3 \cong T\Omega'$, $\widetilde{\nabla}$ is the pull-back via U of the Levi-Civita connection on $T\mathcal{SU}(m)$, R is the curvature $(4,0)$-tensor on $T\mathcal{SU}(m)$, and $\|A\| = (\mathrm{tr}(A^*A))^{1/2}$ is the Hilbert-Schmidt norm in $M_m(\mathbb{C})$.

In order to obtain a convenient stability inequality, we focus on a variational vector field V which is obtained by orthogonal projection onto $T\mathcal{SU}(m)$ of a constant vector field on $M_m(\mathbb{C})$ and we average over such constant vector fields the corresponding inequality given by (A.5). The idea is not new, it is explicitly used in [SU2] when the target is a sphere (averaging over the conformal vector fields) and more generally in [HW] for homogeneous manifolds and *e.g.* in [We] for general targets. Here we follow a very concrete and elementary approach when the target is $\mathcal{SU}(m) \subset M_m(\mathbb{C})$ and we obtain a stability inequality with an explicit constant (see inequality (A.12) below).

Remark A.2. Following [HW] the same inequality (with exactly the same constant) could be deduced in a more abstract way, regarding $\mathcal{SU}(m)$ as a homogeneous (group) manifold. More precisely, one can regard $\mathcal{SU}(m)$ as minimal submanifolds in the sphere $S^{m^2-1}(\sqrt{m})$ through the standard minimal immersion in the first nontrivial eigenspace of its Laplace-Beltrami operator, getting a stability inequality with an explicit constant expressed in terms of the first nonzero eigenvalue of the Laplacian (see e.g. [Xin], pages 137-138 and equation (5.23) or [HW], pages 328-329 and Proposition 5.2). The eigenvalue as well as the dimension of the

(2) Notice that this metric differs by a constant from the metric on $\mathcal{SU}(m)$ induced by the Killing form on $\mathfrak{su}(m)$. The difference is, for our purposes, immaterial.

eigenspace are known in the literature, in terms of the representation theory of the Lie algebra $\mathfrak{su}(m)$, so the constant can be explicitly computed.

To implement this idea, we consider the orthogonal projection $P_U : M_m(\mathbb{C}) \to T_U\mathcal{SU}(m)$ defined by

$$P_U(\phi) = \frac{1}{2} U \left(U^*\phi - \phi^* U - \frac{1}{m} \operatorname{tr}(U^*\phi - \phi^* U)\, \mathbb{I} \right)$$

Clearly, for $U = \mathbb{I}$, the formula above reduces to the orthogonal projection from $M_m(\mathbb{C})$ onto $\mathfrak{su}(m)$. For a fixed $\phi \in M_m(\mathbb{C})$, we define the tangent vector field $\tilde{\phi}^{\mathsf{T}}$ along U by setting

$$\tilde{\phi}^{\mathsf{T}}(k) = P_{U(k)}(\phi).$$

For $\eta \in C_0^\infty(\Omega', \mathbb{R})$, we define $V^{\phi,\eta}(k) := \eta(k)\tilde{\phi}^{\mathsf{T}}(k)$, as a section of the pull-back bundle $U^*T\mathcal{SU}(m)$, corresponding to the admissible variation $U_\varepsilon^{\phi,\eta}(k) = U(k)\exp(\varepsilon\eta(k)U^*(k)\tilde{\phi}^{\mathsf{T}}(k))$. The advantage of this choice is that the second variation of the energy, when averaged with respect to ϕ varying in an orthonormal basis (ONB) of $TM_m(\mathbb{C}) \cong M_m(\mathbb{C})$, decouples as the sum of two simpler terms, as shown in the following lemma.

Lemma A.3. *Let $V^{\phi,\eta}$ be defined as above, and $U_\varepsilon^{\phi,\eta}$ be the corresponding variation. Then*

$$\begin{aligned} \sum_{\phi\in\mathrm{ONB}} \frac{d^2}{d\varepsilon^2}\bigg|_{\varepsilon=0} E(U_\varepsilon^{\phi,\eta};\Omega) &= (m^2-1)\int_\Omega |\nabla\eta|^2 \\ &+ \int_\Omega \eta^2 \sum_j \sum_{\phi\in\mathrm{ONB}} \left\{ \|\widetilde{\nabla}_{e_j}\tilde{\phi}^{\mathsf{T}}\|^2 - R(dU(e_j),\tilde{\phi}^{\mathsf{T}}, dU(e_j),\tilde{\phi}^{\mathsf{T}}) \right\} \end{aligned} \tag{A.6}$$

where the sum runs over ϕ varying in an orthonormal basis of $M_m(\mathbb{C})$.

Proof. By the Leibniz property, for $V \equiv V^{\phi,\eta} = \eta\,\tilde{\phi}^{\mathsf{T}}$ one gets

$$\|\widetilde{\nabla}_{e_j} V\|^2 = |\partial_j\eta|^2\,\|\tilde{\phi}^{\mathsf{T}}\|^2 + 2\,\eta\,\partial_j\eta \left\langle \tilde{\phi}^{\mathsf{T}}, \widetilde{\nabla}_{e_j}\tilde{\phi}^{\mathsf{T}} \right\rangle + \eta^2\,\|\widetilde{\nabla}_{e_j}\tilde{\phi}^{\mathsf{T}}\|^2.$$

We notice that

$$\sum_{\phi\in\mathrm{ONB}} \left\langle \tilde{\phi}^{\mathsf{T}}, \tilde{\phi}^{\mathsf{T}} \right\rangle = \sum_{\phi\in\mathrm{ONB}} \langle \phi\,,\, P_U\phi\rangle = \operatorname{Tr} P_U = \dim \mathcal{SU}(m)$$

where Tr denotes the trace in the algebra $\mathrm{End}(T_U M_m(\mathbb{C}))$ [(3)]. Moreover,

$$\sum_{\phi\in\mathrm{ONB}} \left\langle \tilde{\phi}^{\mathsf{T}}, \widetilde{\nabla}_{e_j}\tilde{\phi}^{\mathsf{T}} \right\rangle = \partial_j \left(\frac{1}{2}\sum_\phi \left\langle \tilde{\phi}^{\mathsf{T}}, \tilde{\phi}^{\mathsf{T}} \right\rangle \right) = \partial_j \left(\frac{1}{2}\dim\mathcal{SU}(m) \right) = 0,$$

so one obtains

$$\sum_{\phi\in\mathrm{ONB}} \sum_j \|\widetilde{\nabla}_{e_j} V\|^2 = \dim\mathcal{SU}(m)\,|\nabla\eta|^2 + \eta^2 \sum_{\phi\in\mathrm{ONB}} \sum_j \|\widetilde{\nabla}_{e_j}\tilde{\phi}^{\mathsf{T}}\|^2.$$

By substituting in (A.5) and recalling that $\dim\mathcal{SU}(m) = m^2-1$ one obtains the claim. □

(3) In contrast, all over the paper we denote by tr the trace in $M_m(\mathbb{C})$, *i.e.* the ordinary matrix trace.

We now exploit the specific structure of $\mathcal{SU}(m)$ to make the last term in (A.6) more explicit. The first lemma does not depend on the particular structure of $V^{\phi,\eta}$, so we state it for any variational vector field V. Hereafter, we set $e_j = \frac{\partial}{\partial k_j}$ and, in view of the embedding $\mathcal{SU}(m) \subset M_m(\mathbb{C})$, we identify $dU(e_j)$ and $\partial_j U$.

Lemma A.4. *Let $V = U\psi$ with $\psi(k) \in \mathfrak{su}(m)$ and $U(k) \in \mathcal{SU}(m)$. Then*

$$\|\widetilde{\nabla}_{e_j} V\|^2 - R(\partial_j U, V, \partial_j U, V) = \|\partial_j \psi\|^2 + \operatorname{tr}\left(U^* \partial_j U \, [\psi, \, \partial_j \psi]\right). \tag{A.7}$$

Proof. The covariant derivative in the pull-back bundle $U^*T\mathcal{SU}(m)$ is equal to the projection on $U^*T\mathcal{SU}(m)$ of the ordinary derivative, *i.e.*

$$\widetilde{\nabla}_{e_j} V(k) = P_{U(k)} \left(\frac{\partial V}{\partial k_j}(k) \right).$$

By an explicit computation, and taking into account that $\psi^* = -\psi$, one gets

$$\widetilde{\nabla}_{e_j} V(k) = U(k) \left(\frac{\partial \psi}{\partial k_j}(k) + \frac{1}{2} \left[U^*(k) \partial_j U(k), \psi(k) \right] \right).$$

Thus, one directly computes

$$\|\widetilde{\nabla}_{e_j} V\|^2 = \|\partial_j \psi\|^2 + \operatorname{tr}\left(U^* \partial_j U \ \left(\psi \, \partial_j \psi^* - \partial_j \psi \, \psi^*\right)\right) + \frac{1}{4} \, \|[U^* \, \partial_j U, \, \psi]\|^2. \tag{A.8}$$

Since $\mathcal{SU}(m)$ is a Lie group with bi-invariant metric $g(A, B) = \operatorname{Re} \operatorname{tr}(A^* B)$ for $A, B \in \mathfrak{su}(m)$, the curvature tensor R can be written in terms of Lie brackets by the *Cartan formula*

$$R(A, B, A, B) = \frac{1}{4} \operatorname{tr}\left([[A, B], A]^* B\right) = \frac{1}{4} \, \|[A, B]\|^2. \tag{A.9}$$

Thus, by left invariance, one has

$$R(\partial_j U, V, \partial_j U, V) = R(U^* \, \partial_j U, \psi, U^* \, \partial_j U, \psi) = \frac{1}{4} \, \|[U^* \partial_j U, \psi]\|^2$$

which cancels exactly the last term in (A.8), yielding the claim. □

Lemma A.5. *With the definitions above, one has*

$$\sum_j \sum_{\phi \in \mathrm{ONB}} \left\{ \|\widetilde{\nabla}_{e_j} \tilde{\phi}^{\intercal}\|^2 - R(\partial_j U, \tilde{\phi}^{\intercal}, \partial_j U, \tilde{\phi}^{\intercal}) \right\} = -\frac{1}{m} \sum_j \|\partial_j U\|^2. \tag{A.10}$$

Proof. By Lemma A.4 applied to $V(k) = \tilde{\phi}^{\intercal}(k)$, one immediately gets

$$\|\widetilde{\nabla}_{e_j} \tilde{\phi}^{\intercal}\|^2 - R(\partial_j U, \tilde{\phi}^{\intercal}, \partial_j U, \tilde{\phi}^{\intercal}) = \|\partial_j \psi\|^2 + \operatorname{tr}\left(U^* \partial_j U \, [\psi, \, \partial_j \psi]\right)$$

where $\psi(k) = U(k)^* \tilde{\phi}^{\intercal}(k)$. By setting

$$\hat{\psi} = \frac{1}{2}(U^* \phi - \phi^* U), \qquad \textit{i.e. } \psi = \hat{\psi} - \frac{1}{m} \operatorname{tr}(\hat{\psi}) \, \mathbb{I},$$

one obtains $\partial_j \psi = \partial_j \hat{\psi} - \frac{1}{m} \operatorname{tr}(\partial_j \hat{\psi}) \, \mathbb{I}$. Since $\partial_j \psi$ and $\mathbb{I}$ are orthogonal in $M_m(\mathbb{C})$,

$$\|\partial_j \psi\|^2 = \|\partial_j \hat{\psi}\|^2 - \frac{1}{m} |\operatorname{tr}(\partial_j \hat{\psi})|^2.$$

We first prove that

$$\sum_{\phi \in \mathrm{ONB}} \frac{1}{m} \,|\operatorname{tr}(\partial_j \hat{\psi})|^2 = \frac{1}{m} \,\|\partial_j U\|^2.$$

Indeed, by the Parseval lemma

$$\begin{aligned}
\sum_{\phi \in \mathrm{ONB}} |\operatorname{tr}(\partial_j \hat{\psi})|^2 &= \sum_{\phi \in \mathrm{ONB}} \frac{1}{4} \left|\operatorname{tr}\left(\partial_j U^* \phi - \phi^* \partial_j U\right)\right|^2 \\
&= \sum_{\phi \in \mathrm{ONB}} \frac{1}{4} \left|2 \operatorname{Re}\operatorname{tr}\left(\phi^*(-i \partial_j U)\right)\right|^2 \\
&= \sum_{\phi \in \mathrm{ONB}} |\left\langle \phi \,,\, -i\partial_j U \right\rangle|^2 = \|\partial_j U\|^2.
\end{aligned}$$

The sum of the remaining terms vanishes, after the summation over an ON basis. Indeed, since $[\psi,\, \partial_j \psi] = [\hat{\psi},\, \partial_j \hat{\psi}]$, one has

$$\operatorname{tr}\left(U^* \partial_j U \,[\psi,\, \partial_j \psi]\right) = \|\partial_j \hat{\psi}\|^2 - \frac{1}{4} \operatorname{tr}\left\{(U^* \partial_j U \phi^* U + U^* \phi U^* \partial_j U)(\partial_j U^* \phi - \phi^* \partial_j U)\right\}.$$

Therefore,

$$\begin{aligned}
&\sum_{\phi \in \mathrm{ONB}} \left\{\|\partial_j \hat{\psi}\|^2 - \operatorname{tr}\left(U^* \partial_j U \,[\psi,\, \partial_j \psi]\right)\right\} \\
&= \sum_{\phi \in \mathrm{ONB}} \frac{1}{4} \operatorname{tr}\left(2\, U^* \partial_j U \phi^* U \partial_j U^* \phi - U^* \partial_j U \phi^* U \phi^* \partial_j U + U^* \phi U^* \partial_j U \partial_j U^* \phi\right). \qquad \text{(A.11)}
\end{aligned}$$

We sum over ϕ in the canonical basis $\{\Phi_{\alpha\beta}, \widetilde{\Phi}_{\alpha\beta}\}$, for $\alpha, \beta \in \{1, \dots, m\}$, where

$$\left[\Phi_{\alpha\beta}\right]_{ab} = \delta_{a\alpha}\delta_{b\beta} \qquad \text{and} \qquad \widetilde{\Phi}_{\alpha\beta} = i\Phi_{\alpha\beta}.$$

Every term in (A.11) in which only ϕ (resp. only ϕ^*) appears, provides a null contribution to the sum over ϕ, since the term containing $\Phi_{\alpha\beta}$ cancels the one containing $\widetilde{\Phi}_{\alpha\beta}$. Therefore,

$$\begin{aligned}
\sum_{\phi \in \mathrm{ONB}} \left\{\|\partial_j \hat{\psi}\|^2 - \operatorname{tr}\left(U^* \partial_j U \,[\psi,\, \partial_j \psi]\right)\right\} &= \frac{1}{2} \sum_{\alpha,\beta} 2 \operatorname{tr}\left(U^* \partial_j U \Phi^*_{\alpha,\beta} U \partial_j U^* \Phi_{\alpha,\beta}\right) \\
&= |\operatorname{tr}(U^* \partial_j U)|^2 = 0,
\end{aligned}$$

where we used that U takes values in $\mathcal{SU}(m)$. □

By the previous lemmas, we obtain the following conclusion.

Proposition A.6 (Stability inequality)**.** *Let $U \in C^\infty(\Omega', \mathcal{SU}(m))$ be a local minimizer of (A.1) in Ω'. Then, for every $\Omega \subset\subset \Omega'$ and every $\eta \in C^\infty_0(\Omega, \mathbb{R})$ one has*

$$\int_\Omega \eta^2 \,\|U^{-1} dU\|^2 \le m(m^2 - 1) \int_\Omega |\nabla \eta|^2. \qquad \text{(A.12)}$$

Proof. We consider the variation $U^{\phi,\eta}_\varepsilon$ corresponding to the variational vector field $V(k) = \eta(k)\tilde{\phi}^{\mathsf{T}}(k)$; by minimality one gets

$$\left.\frac{d^2}{d\varepsilon^2}\right|_{\varepsilon=0} E(U^{\phi,\eta}_\varepsilon; \Omega) \ge 0.$$

By summing over ϕ in an ONB of $M_m(\mathbb{C})$, and taking into account Lemmas A.3, A.4 and A.5 one obtains

$$0 \le \sum_{\phi} \frac{d^2}{d\varepsilon^2}\bigg|_{\varepsilon=0} E(U_\varepsilon^{\phi,\eta};\Omega) = (m^2-1)\int_\Omega |\nabla\eta|^2 - \frac{1}{m}\int_\Omega \eta^2 \sum_j \|\partial_j U\|^2,$$

which by left invariance proves the claim. □

A.2. **Quantization of energy and constancy of tangent maps.** We aim to apply the stability inequality (A.12) to degree-zero homogeneous minimizing harmonic maps (the so-called tangent maps which appear as blow-up limits of a given minimizer when rescaled around a given point, as in Proposition 4.8), in order to show that they are constant.

To prove this property, we restrict ourselves to the case $\Omega' = \mathbb{R}^3 \setminus \{0\}$ and we assume U to be a degree-zero homogeneous harmonic map (so that the determinant will be constant in view of Lemma A.1), i.e. we suppose now that $U(k) = \omega\,(k/|k|)$ for some map $\omega : S^2 \to \mathcal{U}(m)$. If $U \in W^{1,2}_{\mathrm{loc}}(\mathbb{R}^3;\mathcal{U}(m))$ is a local minimizer of (A.1), then ω is a *smooth* harmonic map $\omega \in C^\infty(S^2;\mathcal{U}(m))$ (actually $\omega \in C^\infty(S^2;\mathcal{SU}(m))$ up to multiplication by a constant unitary matrix, in view of Lemma A.1). Indeed, for $m \ge 2$, since U is weakly harmonic and degree-zero homogeneous, then ω is also weakly harmonic, *i.e.* it is a critical point of the energy functional

$$\mathcal{E}(\omega) = \frac{1}{2}\int_{S^2} \left\|\omega^{-1}d\omega\right\|^2 d\mathrm{Vol} \tag{A.13}$$

defined on $W^{1,2}(S^2;\mathcal{U}(m))$. Since any critical point of (A.13) is C^∞-smooth [LW1, Chapter 3], one concludes that ω is C^∞-smooth, as claimed.

Now we take degree-zero homogeneity of U into account. By localizing the inequality (A.12) on S^2, *i.e.* by taking $\eta(k) = \rho(|k|)\psi\,(k/|k|)$ with $\rho \in C_0^\infty((0,\infty))$ and $\psi \in C^\infty(S^2)$ and optimizing in ρ (see [SU2, Lemma 1.3]), one obtains

$$\int_{S^2} |\psi|^2 \frac{1}{2}\left\|\omega^{-1}d\omega\right\|^2 d\mathrm{Vol} \le \frac{1}{2}m(m^2-1)\int_{S^2}\left(|\nabla\psi|^2 + \frac{1}{4}|\psi|^2\right) d\mathrm{Vol}\,. \tag{A.14}$$

In view of the definition (A.13), we set $\psi \equiv 1$ in the previous inequality and we derive the following proposition.

Proposition A.7. *Let $m \ge 2$ and $\omega \in C^\infty(S^2;\mathcal{U}(m))$ an harmonic map. If $U(k) = \omega\left(\frac{k}{|k|}\right)$ is a local minimizer of* (A.1)*, then $\mathcal{E}(\omega) \le \frac{\pi}{2}\, m(m^2-1)$.*

In order to proceed, we recall that a very precise description of the space of all the harmonic maps $\omega \in C^\infty(S^2;\mathcal{U}(m))$ was given in [Uh], proving the so-called factorization into unitons. While the latter paper exploited algebraic techniques, a slightly different factorization result was obtained in [Va], based on an energy induction argument.

Proposition A.8 ([Va], Corollary 7′)**.** *Let $\omega : S^2 \to \mathcal{U}(m)$ be a nonconstant harmonic map. Then there exist a natural number $l \ge 1$ and a canonical factorization*

$$\omega = \omega_0(p_1 - p_1^\perp)\cdots(p_l - p_l^\perp)\,, \quad 8l\pi \le \mathcal{E}(\omega)\,, \tag{A.15}$$

where $\omega_0 \in \mathcal{U}(m)$ and each p_j is the hermitian projection onto a sub-bundle of $S^2 \times \mathbb{C}^m$ holomorphic w.r.to the complex structure induced by the operator $\bar\partial + \bar\partial p_1 + \ldots \bar\partial p_{j-1}$.

Here we regard each projection p_j as a map in a complex Grassmannian $G_{k,m}(\mathbb{C})$, $k = \operatorname{Rank} p_j$, and each factor $p_j - p_j^{\perp}$ in (A.15) as a corresponding map into $\mathcal{U}(m)$, through the isometric embedding $G_{k,m}(\mathbb{C}) \hookrightarrow \mathcal{U}(m)$ (the *Cartan embedding*) defined by assigning to each subspace a unitary operator corresponding the reflection w.r.to the subspace.

The main result in [Va] shows that each factor in (A.15) changes the energy by an integer multiple of 8π. The consequence which will be relevant to us is the following quantization property for a critical point of (A.13).

Proposition A.9 ([Va], Corollary 8)**.** *The energy $\mathcal{E}(\omega)$ of any harmonic map $\omega : S^2 \to \mathcal{U}(m)$ is an integer multiple of 8π. In particular, if ω is noncostant, then $\mathcal{E}(\omega) \geq 8\pi$.*

A straightforward consequence of Propositions A.7 and A.9 is that $\mathcal{E}(\omega) = 0$, and hence ω is constant (and in turn U is constant) whenever $\frac{\pi}{2}\, m(m^2-1) < 8\pi$, *i.e.* for $m = 2$. As already mentioned, this way we recover the regularity property for minimizing harmonic maps into S^3 proved in [SU2, Proposition 1], since $\mathcal{SU}(2) \equiv S^3(\sqrt{2})$.

The case $m = 3$ requires additional care but the conclusion still holds, hence we have the following result.

Corollary A.10. *Let $2 \leq m \leq 3$ and let $U(k) = \omega\left(\frac{k}{|k|}\right)$, $U \in W^{1,2}_{\mathrm{loc}}(\mathbb{R}^3;\mathcal{U}(m))$ be a local minimizer of* (A.1)*. Then U is constant.*

Proof. As already recalled at the beginning of this subsection, $\omega \in C^\infty(S^2;\mathcal{U}(m))$. Since the case $m = 2$ follows readily from Proposition A.7, we assume $m = 3$, and, arguing by contradiction, we may assume $U \not\equiv \text{const}$. By Proposition A.7 we obtain $\mathcal{E}(\omega) \leq 12\pi$, hence $\mathcal{E}(\omega) = 8\pi$ because of Proposition A.9. Going back to Proposition A.8 we see that, up to a constant unitary matrix, we may assume that the product in (A.15) contains only one factor. More precisely, since $S^2 = \mathbb{C}P^1$, $G_{1,3}(\mathbb{C}) = \mathbb{C}P^2$ and, up to isometry, $G_{1,3}(\mathbb{C}) = G_{2,3}(\mathbb{C})$, then $\omega = p - p^{\perp}$, where $p : \mathbb{C}P^1 \to \mathbb{C}P^2$ is an holomorphic map (equivalently, an holomorphic line bundle over $\mathbb{C}P^1$), and $\mathcal{E}(\omega) = 8\pi$.
Now, as in [Va, page 131], let $\tilde{\omega}$ be the Kähler form on $\mathbb{C}P^2$ normalized to be the positive generator in $H^2(\mathbb{C}P^2;\mathbb{Z})$. Then, in homogeneous coordinates $[z_1, z_2] \in \mathbb{C}P^1$, p is a polinomial map of degreee one, since $8\pi|\deg p| = |\int_{\mathbb{C}P^1} p^*\tilde{\omega}| = 8\pi|c_1(p)| = \mathcal{E}(\omega) = 8\pi$, where $c_1(p)$ is the first Chern number of the holomorphic bundle p. As p is nonconstant, $p(z_1, z_2) = [p_1(z_1, z_2),\, p_2(z_1, z_2),\, p_3(z_1, z_2)] \in \mathbb{C}P^2$ for three suitable (not all proportional) degree-one polynomials. Since the degree is one, they are linearly dependent, hence, up to a linear (resp. unitary) change of coordinates on $\mathbb{C}P^2$ (resp. on $\mathbb{C}^3$), we may assume $p_3 \equiv 0$. To summarize, we can regard $p : \mathbb{C}P^1 \to \mathbb{C}P^1 \subset \mathbb{C}P^2$ (the range of p being the set of horizontal lines in $\mathbb{C}^3$) and, up to a further reflection in the third coordinate of $\mathbb{C}^3$, $\omega : S^2 \to \mathcal{U}(2) \subset \mathcal{U}(3)$ through the diagonal embedding (the unitary operator being now the identity on the third coordinate). As we are back to the case $m = 2$, *i.e.* U is a $\mathcal{U}(2)$-valued local minimizer, we conclude $U \equiv \text{const}$, and the contradiction concludes the proof. □

Combining the previous corollary with the well known regularity theory for harmonic maps in three dimension (see [SU1], [Si] and [LW1]) we have the following result which seems to be of independent interest.

Theorem A.11. *Let $2 \leq m \leq 3$ and $\Omega \subset \mathbb{R}^3$ an open set. If $U \in W^{1,2}_{\mathrm{loc}}(\Omega;\mathcal{U}(m))$ is a local minimizer of* (A.1) *then U is real-analytic.*

References

[Bl] Blount, E. I. : Formalism of Band Theory. In : Seitz, F., Turnbull, D. (eds.), *Solid State Physics* **13**, pages 305–373, Academic Press, 1962.

[BZ] Bethuel, F.; Zheng, X.M. : Density of smooth functions between two manifolds in Sobolev spaces. *J. Funct. Anal.* **80** (1988), 60–75.

[BPCM] Brouder Ch.; Panati G.; Calandra M.; Mourougane Ch.; Marzari N.: Exponential localization of Wannier functions in insulators, *Phys. Rev. Lett.* **98** (2007), 046402.

[Ca] Campanato, S. : Proprietà di hölderianità di alcune classi di funzioni. *Ann. Scuola Norm. Sup. Cl. Sci.* **17** (1963), 175–188.

[CaLeLi] Catto I.; Le Bris C.; Lions P.-L.: On the thermodynamic limit for Hartree-Fock type problems, *Ann. I. H. Poincaré* **18** (2001), 687-760.

[CaDeLe] Cancès E.; Deleurence A.; Lewin M. : A New Approach to the Modeling of Local Defects in Crystals: The Reduced Hartree-Fock Case, *Commun. Math. Phys.* **281** (2008), 129–177.

[CWY] Chang, S. Y.; Wang, L.; Yang, P. : Regularity of harmonic maps. *Comm. Pure Appl. Math.* **52** (1999), 1099–1111.

[Cl1] des Cloizeaux, J. : Energy bands and projection operators in a crystal: Analytic and asymptotic properties. *Phys. Rev.* **135** (1964), A685–A697.

[Cl2] des Cloizeaux, J. : Analytical properties of n-dimensional energy bands and Wannier functions. *Phys. Rev.* **135** (1964), A698–A707.

[CLMS] Coifman, R.; Lions, P.-L.; Meyer, Y.; Semmes, S. : Compensated compactness and Hardy spaces. *J. Math. Pures Appl.* **72** (1993), 247–286.

[CNN] Cornean, H.D.; Nenciu A.; Nenciu, G. : Optimally localized Wannier functions for quasi one-dimensional nonperiodic insulators. *J. Phys. A: Math. Theor.* **41** (2008), 125202.

[DuNo] B. A. Dubrovin, S. P. Novikov : Ground state of a two-dimensional electron in a periodic magnetic field, *Zh. Eksp. Teor. Fiz* **79** (1980), 1006-1016. Translated in *Sov. Phys. JETP* **52**, vol. 3 (1980) 511–516.

[Go] Goedecker, S. : Linear scaling electronic structure methods, *Rev. Mod. Phys.* **71** (1999), 1085–1111.

[Ha] Haldane, F.D.M. : Model for a Quantum Hall effect without Landau levels: condensed-matter realization of the "parity anomaly ". *Phys. Rev. Lett.* **61** (1988), 2017.

[HL] Hang, F.; Lin, F.H. : Topology of Sobolev mappings. II. *Acta Math.* **191** (2003), 55–107.

[HS] Helffer, B.; Sjöstrand, J. : Équation de Schrödinger avec champ magnétique et équation de Harper. In: Schrödinger operators, Lecture Notes in Physics 345, Springer, Berlin, 1989, 118–197.

[HW] Howard, R.; Wei, S. W. : Nonexistence of stable harmonic maps to and from certain homogeneous spaces and submanifolds of Euclidean space. *Trans. Amer. Math. Soc.* **294** (1986), 319-331.

[Jo] Jost, J. : Riemannian geometry and geometric analysis. Universitext. Springer, Berlin, 1995.

[Ka] Kato, T. : Perturbation theory for linear operators. Springer, Berlin, 1966.

[Ki] Kievelsen, S. : Wannier functions in one-dimensional disordered systems: application to fractionally charged solitons, *Phys. Rev. B* **26**, 4269–4274 (1982).

[KSV] King-Smith, R. D. ; Vanderbilt, D. : Theory of polarization of crystalline solids, *Phys. Rev. B* **47**, 1651–1654 (1993).

[Ko] Kohn, W. : Analytic Properties of Bloch Waves and Wannier Functions. Phys. Rev. **115**, 809 (1959)

[Ku1] Kuchment, P. : Floquet Theory for Partial Differential Equations. Operator Theory: Advances and Applications. Birkhäuser, 1993

[Ku2] Kuchment, P. : Tight frames of exponentially decaying Wannier functions, *J. Phys. A: Math. Theor.* **42** (2009), 025203.

[Kui] Kuiper, N. : The homotopy type of the unitary group of Hilbert space. *Topology* **3** (1965) 19–30.

[LW1] Lin, F.H.; Wang, C.Y. : The analysis of harmonic maps and their heat flows. World Scientific, 2008.

[LW2] Lin, F.H.; Wang, C.Y. : Stable stationary harmonic maps to spheres. *Acta Math. Sin. (Engl. Ser.)* **22** (2006), 319–330.

[MaVa] Marzari, N. ; Vanderbilt, D.: Maximally localized generalized Wannier functions for composite energy bands. *Phys. Rev. B* **56** (1997), 12847–12865.

[MSV] Marzari, N.; Souza, I.; Vanderbilt, D. An introduction to maximally localized Wannier functions. Highlight of the Month, *Psi-K Newsletter* **57** (2003), 129–168.

[MYSV] Marzari, N.; Mostofi A.A.; Yates J.R.; Souza I.; Vanderbilt D. Maximally localized Wannier functions: Theory and applications, *Rev. Mod. Phys.* **84**, 1419 (2012).

[Mor] Morrey, C.B. : Multiple integrals in the calculus of variations. Grund. der math. Wissenschaften 130. Springer, New York, 1966.

[Mos] Moser, R. : Partial regularity for harmonic maps and related problems. World Scientific, 2005.

[NaMa] Lee, Y.-S.; Nardelli, M. B.; Marzari, N. : Band structure and quantum conductance of nanostructures from maximally localized Wannier functions: the case of functionalized carbon nanotubes *Phys. Rev. Lett.* **95** (2005), 076804.

[Ne1] Nenciu, G. : Existence of the exponentially localised Wannier functions. *Comm. Math. Phys.* **91** (1983), 81–85.

[Ne2] Nenciu, G. : Dynamics of band electrons in electric and magnetic fields: Rigorous justification of the effective Hamiltonians. *Rev. Mod. Phys.* **63** (1991), 91–127.

[NN] Nenciu, A.; Nenciu, G. : The existence of generalized Wannier functions for one-dimensional systems. *Comm. Math. Phys.* **190** (1988), 541–548.

[No] Novikov, S.P. : Magnetic Bloch functions and vector bundles. Typical dispersion law and quantum numbers. *Sov. Math. Dokl.* **23** (1981), 298–303.

[PST] Panati, G.; Spohn, H.; Teufel, S. : Effective dynamics for Bloch electrons: Peierls substitution and beyond. *Comm. Math. Phys.* **242** (2003), 547–578.

[Pa] Panati, G.: Triviality of Bloch and Bloch-Dirac bundles. *Ann. Henri Poincaré* **8** (2007), 995–1011.

[Pr] Prodan, E. : Disordered topological insulators: a Non-Commutative Geometry perspective. *J. Phys. A: Math. Theor.* **44** (2011), 113001.

[RS] Reed M., Simon, B. : Methods of Modern Mathematical Physics. Volume IV: Analysis of Operators. Academic Press, New York, 1978.

[Re] Resta, R. : Theory of the electric polarization in crystals, *Ferroelectrics* **136**, 51–75 (1992).

[Si] Simon, L. : Theorems on regularity and singularity of energy minimizing maps. Lectures in Mathematics ETH Zürich. Birkhäuser, Basel, 1996.

[St] Stein, E. : Harmonic analysis: real-variable methods, orthogonality, oscillatory integrals. Princeton Mathematical Series, 43. Princeton University Press, Princeton, 1993.

[SU1] Schoen, R.; Uhlenbeck, K. : A regularity theory for harmonic maps. *J. Differential Geom.* **17** (1982), 307–335.

[SU2] Schoen, R.; Uhlenbeck, K. : Regularity of minimizing harmonic maps into the sphere. *Invent. Math.* **78** (1984), 89–100.

[TCVR] Thonhauser, T.; Ceresoli, D.; Vanderbilt, D.; Resta, R. : Orbital magnetization in periodic insulators, *Phys. Rev. Letters* **95** (2005), 137205.

[Uh] Uhlenbeck, K.: Harmonic maps into Lie groups: classical solutions of the chiral model. *J. Differential Geom.* **30** (1989), 1–50.

[Va] Valli, G.: On the energy spectrum of harmonic 2-spheres in unitary groups. *Topology* **27** (1988), 129–136.

[Wa] Wannier, G. H. : The structure of electronic excitation levels in insulating crystals. *Phys. Rev.* **52** (1937), 191–197.

[We] Wei, W.: Liouville Theorems for stable harmonic maps into either strongly unstable, or $\delta-$pinched manifolds. *Proceedings of Symposia in Pure Mathematic* **44** (1986).

[Xin] Xin, Y.L.: Geometry of harmonic maps. Progress in Nonlinear Differential Equations and their Applications, 23. Birkhäuser, Boston, 1996.

(G. Panati) Dipartimento di Matematica "G. Castelnuovo", "La Sapienza" Università di Roma, Piazzale A. Moro 2, 00185 Roma, Italy

E-mail address: panati@mat.uniroma1.it

(A. Pisante) Dipartimento di Matematica "G. Castelnuovo", "La Sapienza" Università di Roma, Piazzale A. Moro 2, 00185 Roma, Italy

E-mail address: pisante@mat.uniroma1.it