Ann. Henri Poincaré 8 (2007), 995–1011

1424-0637/050995-17, *published online* July 16, 2007
DOI 10.1007/s00023-007-0326-8

Annales Henri Poincaré

Triviality of Bloch and Bloch–Dirac Bundles

Gianluca Panati

Abstract. In the framework of the theory of an electron in a periodic potential, we reconsider the longstanding problem of the existence of smooth and periodic quasi-Bloch functions, which is shown to be equivalent to the triviality of the Bloch bundle. By exploiting the time-reversal symmetry of the Hamiltonian and some bundle-theoretic methods, we show that the problem has a positive answer in any dimension $d \leq 3$, thus generalizing a previous result by G. Nenciu. We provide a general formulation of the result, aiming at the application to the Dirac equation with a periodic potential and to piezoelectricity.

1. Introduction

Many relevant properties of crystalline solids can be understood by the analysis of Schrödinger operators in the form

$$H = -\Delta + V_\Gamma\,, \tag{1}$$

where the potential $V_\Gamma : \mathbb{R}^d \to \mathbb{R}$ is periodic with respect to a lattice $\Gamma \subset \mathbb{R}^d$. Here by *lattice* we mean a maximal discrete subgroup of the group $(\mathbb{R}^d, +)$, thus $\Gamma \cong \mathbb{Z}^d$. As realized at the dawn of quantum mechanics, the analysis of operators in the form (1) is greatly simplified by the use of the Bloch–Floquet transform, here denoted as $\mathcal{U}_{\mathrm{B}}$. The advantage of this construction is that the transformed Hamiltonian $\mathcal{U}_{\mathrm{B}}\, H\, \mathcal{U}_{\mathrm{B}}^{-1}$ is a fibered operator with respect to a parameter $k \in \mathbb{T}^d$ (called *crystal momentum* or *Bloch momentum*) and that, under very general assumptions on V_Γ, each fiber operator $H(k)$ has compact resolvent and thus pure point spectrum accumulating at infinity. We label the eigenvalues in increasing order, i.e., $E_0(k) \leq E_1(k) \leq \dots$ The function E_n is called the n-th *Bloch band*.

In many applications one is interested in a family of orthogonal projectors $\{P(k)\}_{k\in\mathbb{T}^d}$, where $P(k)$ is the spectral projector of $H(k)$ corresponding to a Bloch band, or to a family of Bloch bands, which is separated (pointwise in k) by a gap from the rest of the spectrum. As a particular but important case, one may consider the spectral projector up to the Fermi energy E_{F}, assuming that the latter lies in an energy gap for all k, a situation which is relevant when considering the polarization properties of insulators and semiconductors. Since the map $k \mapsto H(k)$ is periodic and smooth (in the norm-resolvent sense), the same is true for the map $k \mapsto P(k)$. Moreover, in many cases, $P(k)$ is indeed analytic over a complex strip $\mathcal{T}_a = \{k \in \mathbb{C}^d : |\operatorname{Im} k_i| < a\}$. Thus one may raise the following question:

Question (A): is it possible to choose a system $\{\varphi_a(k)\}_{a=1,\dots,m}$ of eigenfunctions of $P(k)$, spanning $\operatorname{Ran} P(k)$, such that the maps $k \mapsto \varphi_a(k)$ are smooth (resp. analytic) and periodic?

The special case $m = 1$ (i.e., when $P(k)$ is the spectral projector corresponding to a non-degenerate band E_n) corresponds to an old problem in solid state physics, namely the existence of smooth and periodic Bloch functions. Indeed, the solution of the eigenvalue problem

$$H(k)\psi_n(k) = E_n(k)\psi_n(k)\,, \tag{2}$$

yields a Bloch function $\psi_n(k)$ which is defined only up to a k dependent phase. Clearly one can always choose the phase in such a way that $\psi_n(k)$ is *locally* smooth in k, but it is not clear a priori if such local solutions can be glued together to obtain a smooth and periodic function. A geometrical obstruction might appear. For example, if one includes a magnetic field in the Hamiltonian (thus breaking time-reversal symmetry) it turns out that Question (A) has in general a negative answer, even in the smooth case [6, 12, 18].

As for the time-symmetric Hamiltonian (1), G. Nenciu proved that the question has a positive answer, in the analytic sense, if $m = 1$ or, alternatively, $d = 1$ ([17], see also [15] Theorem 3.5 and references therein). An alternative proof has been later provided by Helffer and Sjöstrand [9].

On the other side, in dimension $d = 3$ the case of a non-degenerate Bloch band globally isolated from the rest of the spectrum is not generic. It is more natural to consider rather a family of Bloch bands which may cross each other, which means to deal with the case $m > 1$.

In this paper we show that Question (A) has a positive answer in the analytic sense for any $m \in \mathbb{N}$, provided that $d \leq 3$ and that the Hamiltonian satisfies time-reversal symmetry. Borrowing the terminology introduced in [5], this can be rephrased by saying that we prove the existence of analytic and periodic *quasi-Bloch functions.*

The result is extremely important for condensed matter physics. Indeed, as pointed out in [3], the existence of analytic and periodic quasi-Bloch functions is the crucial step to prove the existence of exponentially localized Wannier functions in insulators, one of the oldest and longstanding problems in the theory of solids [13, 15, 25]. Notice that the description of an insulator by an orthonormal and localized basis is a crucial issue, since it allows for the development of computational methods scaling linearly with the system size [8] and it yields a more familiar understanding of the physics in term of tight-binding hamiltonians with short range parameters.

Moreover, a positive answer in the case $m > 1$ is relevant for a rigorous derivation of the semiclassical model of solid state physics [20], for the analysis of piezoelectricity in crystalline solids [19], and for the derivation of an effective Hamiltonian for particles with spin degrees of freedom in a periodic environment, e.g., the Pauli equation or the Dirac equation with periodic potential [14].

While previous proofs (for the case $m = 1$ or $d = 1$) exploit operator-theoretic techniques, our strategy is to reformulate the problem in a geometric language, as suggested, but non substantiated, in [15]. After reformulating the problem in the context of bundle theory, we use Steenrod's classification theory [23] and some ideas in [1] in order to solve it. It is our belief that mathematical physics greatly benefits from the interplay between analytic and geometric techniques, and we hope that this result illustrates this viewpoint.

A relevant advantage of the geometric method is that one does not loose information about the size of the analyticity strip. On the other side, the proof is not explicitly constructive.

Finally, we mention in parenthesis that even for non-periodic systems one may introduce generalized Wannier functions, defined as eigenfunctions of the "band position operator". This viewpoint, which traces back to [11], has been mathematically substantiated in [16].

In Section 2 we state and prove our main results, which are then applied to the specific case of Schrödinger operators in Section 3 and to Dirac operators in Section 4.

2. The main result

2.1. Assumptions and statements

It is convenient to abstract from the specific context of Schrödinger–Bloch operators, and to state the result in a general framework. Hereafter, we denote as $\mathcal{B}(\mathcal{H})$ the algebra of bounded operators over a separable Hilbert space $\mathcal{H}$, and with $\mathcal{U}(\mathcal{H})$ the group of unitary operators over $\mathcal{H}$. In the application to Schrödinger operators, the lattice Λ which appears below will be identified with Γ^*.

Assumption (P). *Let Λ be a maximal lattice in $\mathbb{R}^d$. We assume that $\{P(k)\}_{k\in\mathbb{R}^d}$ is a family of orthogonal projectors acting on a separable Hilbert space $\mathcal{H}$, such that*

(P_1) *the map $k \mapsto P(k)$ is smooth from $\mathbb{R}^d$ to $\mathcal{B}(\mathcal{H})$*

(P_2) *the map $k \mapsto P(k)$ is covariant with respect to a unitary representation of the group Λ, in the sense that*

$$P(k+\lambda) = \tau(\lambda)^{-1}\, P(k)\, \tau(\lambda) \qquad \forall k \in \mathbb{R}^d,\ \forall \lambda \in \Lambda\,,$$

where $\tau : \Lambda \to \mathcal{U}(\mathcal{H})$ is a group homomorphism.

We are now in position to state our main result.

Theorem 1. *Let Λ be a maximal lattice in $\mathbb{R}^d$. Let $\{P(k)\}_{k\in\mathbb{R}^d}$ be a family of orthogonal projectors acting on a separable Hilbert space $\mathcal{H}$, satisfying Assumption* (P) *and moreover:*

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

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

Let $m := \dim P(k)$ and assume $d \leq 3, m \in \mathbb{N}$ or, alternatively, $d \geq 4, m = 1$. Then each of the following equivalent properties holds true:

(A) **existence of global (quasi-)Bloch functions:** *there exists a collection of smooth maps $k \mapsto \varphi_a(k)$ (indexed by $a = 1, \ldots, m$) from $\mathbb{R}^d$ to $\mathcal{H}$ such that:*
  (A_1) *the family $\{\varphi_a(k)\}_{a=1}^m$ is an orthonormal basis spanning* $\mathrm{Ran}P(k)$*;*
  (A_2) *each map is τ-equivariant in the sense that*

$$\varphi_a(k+\lambda) = \tau(\lambda)^{-1}\varphi_a(k) \qquad \forall k \in \mathbb{R}^d,\ \forall \lambda \in \Lambda\,.$$

(B) **existence of an intertwining unitary:** *there exists a smooth map $k \mapsto U(k)$ from $\mathbb{R}^d$ to $\mathcal{U}(\mathcal{H})$ such that:*
  (B_1) *each $U(k)$ intertwines* $\mathrm{Ran}\,P(0)$ *and* $\mathrm{Ran}\,P(k)$*,*

$$U(k)^*\,P(k)\,U(k) = P(0) \qquad \forall k \in \mathbb{R}^d\,;$$

  (B_2) *the correspondence is τ-equivariant in the sense that:*

$$U(k+\lambda) = \tau(\lambda)^{-1}\,U(k) \qquad \forall k \in \mathbb{R}^d,\ \forall \lambda \in \Lambda\,.$$

It is convenient to reformulate properties (A) and (B) in a bundle-theoretic language, by introducing the complex vector bundle canonically associated to the family $\{P(k)\}_{k\in\mathbb{R}^d}$. More formally, for any family of projectors satisfying Assumption (P), we define a hermitian complex vector bundle ϑ in the following way. First one introduces on the set $\mathbb{R}^d \times \mathcal{H}$ the equivalence relation $\sim_\tau$, where

$$(k,\varphi) \sim_\tau (k',\varphi') \qquad \Leftrightarrow \qquad (k',\varphi') = \big(k+\lambda\,,\,\tau(\lambda)\varphi\big) \quad \text{for some } \lambda \in \Lambda\,.$$

The equivalence class with representative (k,φ) is denoted as $[k,\varphi]$. Then the total space E of the bundle ϑ is defined as

$$E := \big\{[k,\varphi] \in (\mathbb{R}^d \times \mathcal{H})/\!\sim_\tau \,:\, \varphi \in \mathrm{Ran}\,P(k)\big\}\,.$$

This definition does not depend on the representative in view of the covariance property (P_2). The base space is the flat torus $B := \mathbb{R}^d/\Lambda$ and the projection to the base space $\pi : E \to B$ is $\pi[k,\varphi] = \mu(k)$, where μ is the projection modulo Λ, $\mu : \mathbb{R}^d \to B$. One checks that $\vartheta = (E \xrightarrow{\pi} B)$ is a smooth complex vector bundle with typical fiber $\mathbb{C}^m$. In particular, the local triviality follows, for example, from (P_1) and the use of the Nagy formula[2].

[1] By *antiunitary* operator we mean an 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 $\varphi, \psi \in \mathcal{H}$.

[2] Indeed, for any $k_0 \in \mathbb{R}^d$ there exist a neighbourhood $\mathcal{W} \subset \mathbb{R}^d$ of k_0 such that $\|P(k) - P(k_0)\| < 1$ for any $k \in \mathcal{W}$. Then by posing (Nagy's formula)

$$W(k) := \Big(\big(1-(P(k)-P(k_0))^2\big)\Big)^{-1/2}\Big(P(k)P(k_0) + \big(1-P(k)\big)\big(1-P(k_0)\big)\Big)$$

Moreover the vector bundle ϑ carries a natural hermitian structure. Indeed, if $v_1, v_2 \in E$ are elements of the fiber over $x \in B$, then up to a choice of the representatives

$$v_1 = [x, \varphi_1] \quad \text{and} \quad v_2 = [x, \varphi_2]\,,$$

and one poses

$$\langle v_1, v_2 \rangle_{E_x} := \langle \varphi_1, \varphi_2 \rangle_{\mathcal{H}} \,.$$

Endowed with this hermitian structure ϑ is turned into a G-bundle with structural group $G = U(m)$.

Proposition 2. *Under the same assumptions as in Theorem* 1*, the properties* (A) *and* (B) *are equivalent to:*

(C) **triviality of the corresponding vector bundle:** *the vector bundle associated to the family $\{P(k)\}_{k\in\mathbb{R}^d}$ according to the previous construction is trivial in the category of smooth $U(m)$-bundles over B.*

Proof. (**A**) $\Leftrightarrow$ (**C**). Property (A) claims that the bundle ϑ admits a global smooth orthonormal frame, i.e., that the principal bundle associated to ϑ (i.e., the *bundle of frames* in the physics language) admits a global smooth section. The latter claim is equivalent to the triviality of ϑ in the category of smooth $U(m)$-bundles over B, namely property (C).

(**A**) $\Leftrightarrow$ (**B**). Assume property (B). If $\{\chi_a\}_{a=1,\dots,m}$ is any orthonormal basis of $\operatorname{Ran} P(0)$, then $\varphi_a(k) := U(k)\chi_a$, for $a = 1,\dots,m$, satisfies condition (A). Viceversa, assume $\{\varphi_a\}_a$ satisfies property (A). Then by posing

$$W(k)\psi = \sum_a \langle \varphi_a(0),\, \psi\rangle_{\mathcal{H}}\, \varphi_a(k)$$

one defines a partial isometry from $\operatorname{Ran} P(0)$ to $\operatorname{Ran} P(k)$. The orthogonal projection $Q(k) := 1 - P(k)$ satisfies assumptions (P_1)-(P_3) too, since $C^2 = 1$. Thus, by the same argument as before one gets a partial isometry $Y(k)$ intertwining $\operatorname{Ran} Q(0)$ and $\operatorname{Ran} Q(k)$. By di rect sum one gets a unitary operator $U(k) = W(k) \oplus Y(k)$ which satisfies property (B). $\square$

The proof of Theorem 1 is based on the following scheme. In the first part, by using standard ideas, one shows that hypothesis (P_3) (which corresponds to *time-reversal symmetry* in the applications) implies that the trace of the curvature of the Berry connection of ϑ has a special property, namely $\Omega(-k) = -\Omega(k)$. Thus the first Chern class of ϑ vanishes. The difficult step is to show that this condition is *sufficient* for the triviality of the bundle ϑ. The latter claim, whose proof is based on Proposition 4, relies on the special structure and the low-dimensionality of the base space $B \approx \mathbb{T}^d, d \leq 3$. (In this paper the symbol $\approx$ denotes homeomorphism of topological spaces)

---

one gets a smooth map $W : \mathcal{W} \to \mathcal{U}(\mathcal{H})$ such that $W(k)\,P(k)\,W(k)^{-1} = P(k_0)$. If $\{\chi_a\}_{a=1,\dots,m}$ is any orthonormal basis spanning $\operatorname{Ran}P(k_0)$, then $\varphi_a(k) = W(k)\chi_a$ is a smooth local orthonormal frame for ϑ.

By the *Oka's principle*, the result can be pushed forward to the analytic category, yielding the following "corollary".

Theorem 3. *Let* $\mathcal{T}_a = \{z \in \mathbb{C}^d : |\,\mathrm{Im} z_i\,| < a, \forall i = 1, \ldots, d\}$ *for a fixed* $a > 0$ *and* Λ *a maximal lattice in* $\mathbb{R}^d$*, regarded as a subset of* $\mathbb{C}^d$*. Let* $\{P(z)\}_{z \in \mathcal{T}_a}$ *be a family of orthogonal projectors in* $\mathcal{H}$*, satisfying*

($\widetilde{\mathrm{P}}_1$) *the map* $z \mapsto P(z)$ *is* analytic *from* $\mathcal{T}_a$ *to* $\mathcal{B}(\mathcal{H})$;

($\widetilde{\mathrm{P}}_2$) *the map* $z \mapsto P(z)$ *is* τ*-covariant, in the sense that*

$$P(z+\lambda) = \tau(\lambda)^{-1}\, P(z)\, \tau(\lambda) \qquad \forall z \in \mathcal{T}_a,\ \forall \lambda \in \Lambda\,,$$

where $\tau : \Lambda \to \mathcal{U}(\mathcal{H})$ *is a group homomorphism;*

($\widetilde{\mathrm{P}}_3$) *there exists an antiunitary operator* C *acting on* $\mathcal{H}$ *such that* $C^2 = 1$ *and* $P(-z) = C\, P(z)\, C$ *for all* $z \in \mathcal{T}_a$.

Let $m := \dim P(z)$ *and assume* $d \le 3, m \in \mathbb{N}$ *or, alternatively,* $d \ge 4, m = 1$*. Then each of the following equivalent properties holds true:*

(A) *there exists a collection of* analytic *functions* $z \mapsto \varphi_a(z)$ (*indexed by* $a = 1, \ldots, m$) *from* $\mathcal{T}_a$ *to* $\mathcal{H}$ *satisfying* (A_1) *and* (A_2) *over* $\mathcal{T}_a$*;*

(B) *there exists an* analytic *function* $z \mapsto U(z)$ *from* $\mathcal{T}_a$ *to* $\mathcal{U}(\mathcal{H})$ *satisfying* (B_1) *and* (B_2) *over* $\mathcal{T}_a$.

Notice that Theorem 3 provides a complete answer, for $d \le 3$, to the question raised in [17]. A similar statement holds true if the map $z \mapsto P(z)$ satisfy the symmetry

$$P(-\bar{z}) = CP(z)C \;\forall z \in \mathcal{T}_a\,, \tag{3}$$

where $\bar{z}$ denotes the complex conjugate of z.

2.2. Proof of main results

Proof of Theorem 1. Let Ω be the differential 2-form over $\mathbb{R}^d$ with components

$$\Omega_{i,j}(k) = \mathrm{Tr}\left(P(k)\left[\partial_i P(k),\, \partial_j P(k)\right]\right)$$

i.e.,

$$\Omega(k) = \sum_{i,j} \Omega_{i,j}(k)\, dk^i \wedge dk^j. \tag{4}$$

In view of property (P_2), Ω is Λ-periodic, and thus defines a 2-form over B. We are going to show how Ω is related to the curvature of a connection over the vector bundle ϑ.

By using a local frame $\Psi = (\psi_1, \ldots, \psi_m)$ over $\mathcal{W} \subset \mathbb{R}^d$, one defines locally a 1-form $\mathcal{A}(k) = \sum_i \mathcal{A}_i(k) dk^i$ with coefficients $\mathcal{A}_i(k)$ in $\mathfrak{u}(m)$, the Lie algebra of antihermitian matrixes, given by[3]

$$\mathcal{A}_i(k)_{ab} = \left\langle \psi_a(k), \partial_i \psi_b(k)\right\rangle, \quad k \in \mathcal{W}\,. \tag{5}$$

[3]Here and in the following $i, j, \ldots \in \{1, \ldots, d\}$ are the base-space indexes, while $a, b, c \in \{1, \ldots, m\}$ are the matrix (Lie algebra) indexes.

It is easy to check how $\mathcal{A}$ transforms under a change of local trivialization: if $\widetilde{\Psi} = (\tilde{\psi}_1, \dots, \tilde{\psi}_m)$ is a local trivialization over $\tilde{\mathcal{W}}$, such that $\Psi(k) = G(k)\tilde{\Psi}(k)$ for a smooth $G : \mathcal{W} \cup \widetilde{\mathcal{W}} \to U(m)$, then the 1-form $\mathcal{A}$ transforms as

$$\widetilde{\mathcal{A}_i}(k) = G(k)^{-1}\, \mathcal{A}_i(k)\, G(k) + G(k)^{-1}\, dG(k) \qquad k \in \mathcal{W} \cap \widetilde{\mathcal{W}} . \tag{6}$$

The transformation property (6) implies (see [2], Theorem 1.2.5) that $\mathcal{A}$ is the local expression of a $U(m)$-connection over the complex vector bundle ϑ. (Such a connection is called *Berry connection* in the physics literature. Mathematically, it is the connection induced by the embedding of ϑ in the trivial hermitian bundle $B \times \mathcal{H}_{\mathrm{f}} \to B$).

A lengthy but straightforward computation yields

$$\Omega_{i,\,j} = \mathrm{tr}\,(\partial_i \mathcal{A}_j - \partial_j \mathcal{A}_i + \mathcal{A}_i\, \mathcal{A}_j - \mathcal{A}_j\, \mathcal{A}_i)$$

where tr denotes the trace over the matrix (Lie algebra) indexes. Thus one concludes that $\Omega = \mathrm{tr}\, \omega_{\mathcal{A}}$, where

$$\omega_{\mathcal{A}} := d\mathcal{A} + \mathcal{A} \wedge \mathcal{A}$$

represents locally the curvature of the connection $\mathcal{A}$. Therefore the first real Chern class of the bundle ϑ is

$$\mathrm{Ch}_1(\vartheta) = \frac{i}{2\pi}\, [\mathrm{tr}\, \omega_{\mathcal{A}}] = \frac{i}{2\pi}\, [\Omega] ,$$

where $[\dots]$ denotes the de Rahm cohomology class.

By property (P_3) one has that $\partial_i P(-k) = -C\, \partial_i P(k)\, C$, thus

$$\begin{aligned} \Omega_{i,j}(-k) &= \mathrm{Tr}\, \Big(C\, P(k) C\, C \left[\partial_i P(k),\, \partial_j P(k) \right] C \Big) \\ &= -\,\mathrm{Tr}\, \Big(P(k) \left[\partial_i P(k),\, \partial_j P(k) \right] \Big) \\ &= -\Omega_{i,j}(k) , \end{aligned}$$

where we used the fact that $\mathrm{Tr}(C\, A\, C) = \mathrm{Tr}(A^*)$ for any $A \in \mathcal{B}(\mathcal{H})$. Thus one concludes that

$$\Omega(-k) = -\Omega(k) . \tag{7}$$

It follows from (7) that the first *real* Chern class of ϑ vanish. Indeed, in $B \approx \mathbb{T}^d$ equipped with periodic coordinates $k = (k_1, \dots, k_d)$, $k_i \in [-\pi, \pi)$, one considers the 2-cycles defined by the sets

$$\Theta_{j,l} := \left\{ k \in \mathbb{T}^d : k_i = 0 \text{ for any } i \notin \{j, l\} \right\} , \quad \text{for } \ j, l = 1, \dots, d,\ j \neq l , \tag{8}$$

with any consistent choice of the orientation. From (7) it follows that

$$\frac{i}{2\pi} \int_{\Theta_{j,l}} \Omega = 0 . \tag{9}$$

It remains to show that the independent cycles $\{\Theta_{j,l}\}_{j \neq l}$ are a basis for $H_2(\mathbb{T}^d, \mathbb{R})$. Indeed, from Künneth formula one proves by induction that $H_2(\mathbb{T}^d, \mathbb{Z}) \cong \mathbb{Z}^{k(d)}$ with $k(d) = \frac{1}{2} d(d-1)$. Therefore, the independent 2-cycles $\Theta_{j,l}$ generate, by linear combinations with coefficients in $\mathbb{Z}$ (resp. $\mathbb{R}$), all $H_2(\mathbb{T}^d,\mathbb{Z})$ (resp. $H_2(\mathbb{T}^d,\mathbb{R})$). Thus, by de Rham's isomorphism theorem, from (9) it follows that $\mathrm{Ch}_1(\vartheta)=0$.

We conclude that the first *real* Chern class of the bundle ϑ vanishes. Since the natural homomorphism $H^2(\mathbb{T}^d,\mathbb{Z}) \to H^2(\mathbb{T}^d,\mathbb{R})$ is injective, this implies the vanishing of the first *integer* Chern class.

As for $m=1$, it is a classical result by Weil and Constant ([26], see also [4] Theorem 2.1.3) that the vanishing of the first integer Chern class of a complex line bundle over a (paracompact) manifold implies the triviality of the bundle itself. For $m \geq 2$, it follows from Proposition 4 that for a base space $B \approx \mathbb{T}^d$ with $d \leq 3$ the vanishing of the first real Chern class implies the triviality of the bundle ϑ, i.e., property (C). This concludes the proof of the theorem. □

Proof of Theorem 2. In strict analogy with the smooth case, the problem is equivalent to the triviality (in the analytic category) of an analytic $U(m)$-bundle $\tilde{\vartheta}$ over the open poly-cylinder $\mathcal{T}_a/\Lambda$. Since there exists a deformation retract $\rho : \mathcal{T}_a/\Lambda \to \mathbb{T}^d$ the triviality of the bundle $\tilde{\vartheta}$ (in the smooth sense) is equivalent to the triviality of its retraction over $\mathbb{T}^d$. Then the proof of Theorem 1 implies that $\tilde{\vartheta}$ is trivial in the category of *smooth* $U(m)$-bundles over $\mathcal{T}_a/\Lambda$.

By the Oka principle (see [7], Chapter V) if an analytic bundle over a Stein manifold is topologically trivial, then it is analytically trivial. This result applies to our case, since $\mathcal{T}_a/\Lambda$ is the cartesian product of non-compact Riemann surfaces, and as such a Stein manifold. □

2.3. A technical lemma

We prove in this section a technical result used in the proof of Theorem 1, which shows that when the base space is a low dimensional torus (or, more generally, any low dimensional connected compact manifold whose second cohomology is torsionless) the vanishing of the first real Chern class of a $U(m)$-bundle implies the triviality of the bundle itself. The proof is based on Steenrod's classification theory [23] and on some ideas in the literature [1].

We first recall ([22] Section 5.9) that there is a natural transformation $i : H^2(\cdot,\mathbb{Z}) \to H^2(\cdot,\mathbb{R})$, so that for any $f : X \longrightarrow Y$ the following diagram is commutative:

$$\begin{tikzcd} H^2(X,\mathbb{Z}) \arrow[d, "i_X"'] & H^2(Y,\mathbb{Z}) \arrow[l, "f^*"'] \arrow[d, "i_Y"'] \\ H^2(X,\mathbb{R}) & H^2(Y,\mathbb{R}) \arrow[l, "f^*"'] \end{tikzcd}$$

When one specialize to $X \cong \mathbb{T}^d$, the natural homomorphism $i : H^2(\mathbb{T}^d,\mathbb{Z}) \to H^2(\mathbb{T}^d,\mathbb{R})$ is injective.

We denote as $k_G(X)$ the set of vertical isomorphism classes of principal smooth G-bundles over X (see [10], Section 4.10). By vertical isomorphism we mean an isomorphism which projects over the identity map on X, i.e., reshuffling of the fibers is not allowed.

Proposition 4. *If X is a compact, connected manifold of dimension $d \leq 3$ and $G = U(m)$ for $m \geq 2$, then $k_G(X) \cong H^2(X, \mathbb{Z})$, where the isomorphism (of pointed sets) is realized by first integer Chern class. In particular, if X is such that the natural homomorphism $H^2(X, \mathbb{Z}) \to H^2(X, \mathbb{R})$ is injective, then for any $U(m)$-bundle ϑ over X the vanishing of the first* real *Chern class* $\mathrm{Ch}_1(\vartheta)$ *implies the triviality of ϑ.*

For sake of a more readable proof, we first recall some results about the classification theory of G-bundles [23]. A principal G-bundle $\Upsilon_G = (E_G \overset{p_G}{\to} B_G; G)$ is said to be *universal* if the map $[X, B_G] \to k_G(X)$, which associate to a (free) homotopy class of maps $[f]$ the isomorphism class of the pull-back bundle $f^*\Upsilon$, is a bijection for all X. A principal G-bundle with total space P is universal if and only if P is contractible, and for any finite-dimensional Lie group G there exists a universal G-bundle. The base spaces of different universal G-bundles for the same group G are homotopically equivalent.

We also make use in the proof of the Eilenberg–Mac Lane spaces (see [22], Sect. 8.1). We recall that for any $n \in \mathbb{N}$ and any group π (abelian if $n \geq 2$) there exists a path connected space Y such that $\pi_k(Y) = \pi$ for $k = n$ and zero otherwise. This space is unique in the category of CW-complexes and denoted by $K(\pi, n)$.

Proof. From abstract classification theory we know that $k_G(X) \cong [X, B_G]$, but unfortunately a simple representation of $[X, B_G]$ is generally not available. The crucial observation [1] is that if we are interested only in manifolds with $\dim X \leq n$ the homotopy groups of B_G beyond the n^{th} do not play any role, therefore one can "approximate" B_G with a space B_3 which captures the relevant topological features of B_G.

More precisely, one constructs a space B_3 which is 4-equivalent to B_G, in the sense that there exist a continuous map

$$\rho : B_G \longrightarrow B_3$$

such that

$$\pi_k(\rho) : \pi_k(B_G) \longrightarrow \pi_k(B_3)$$

is an isomorphism for $k \leq 3$ and a epimorphism for $k = 4$. Therefore, for any complex X of dimension $d \leq 3$, one has $[X, B_G] = [X, B_3]$.

From the exact homotopy sequence of the universal bundle Υ one has $\pi_k(B_G) = \pi_{k-1}(G)$, so that for $G = U(m)$ one has

(i) $\pi_1(B_G) = \pi_0(G) = 0$,
(ii) $\pi_2(B_G) = \pi_1(G) = \mathbb{Z}$,
(iii) $\pi_3(B_G) = \pi_2(G) = 0$.

Since B_G is simply connected, there is already a 2-equivalence

$$\rho : B_G \longrightarrow B_3 := K(\mathbb{Z}, 2) \approx \mathbb{C}P^\infty$$

see [22]. Since $\pi_3(B_G) = 0$, $\pi_3(\rho)$ is an isomorphism, and $\pi_4(\rho)$ is surjective since $\pi_4(K(\mathbb{Z}, 2)) = 0$. Therefore ρ is a 4-equivalence, so that

$$k_G(X) \cong [X, K(2, \mathbb{Z})] \cong H^2(X, \mathbb{Z}) .$$

The first identification is an isomorphism of pointed sets, i.e., the trivial element $[f] \in [X, K(2, \mathbb{Z})]$ corresponds to the (equivalence class of) the trivial $U(m)$-bundle over X. As for the second, let be η any non zero element of $H^2(\mathbb{C}P^\infty, \mathbb{Z})$. Then, according to [22] Theorem 8.1.8, the map

$$\begin{array}{rccc} \psi_X : & [X, K(2, \mathbb{Z})] & \to & H^2(X, \mathbb{Z}) \\ & [f] & \mapsto & f^*\eta \end{array}$$

is an isomorphism of pointed sets. Consider now the following diagram

$$\begin{tikzcd} {[X, K(2, \mathbb{Z})]} \arrow[r, "\psi_X"] \arrow[d] & H^2(X, \mathbb{Z}) \arrow[d, "i_X"] \\ k_G(X) \arrow[ur, "\mathrm{ch}_1"] \arrow[r, "\mathrm{Ch}_1"] & H^2(X, \mathbb{R}) \end{tikzcd}$$

where the diagonal arrow represents the first integer Chern class. The lower tringle is commutative since $\mathrm{Ch}_1 = i \circ \mathrm{ch}_1$. As for the upper triangle, one choose $\eta := \mathrm{ch}_1(\Upsilon_G)$ which is certainly not zero. Then, since

$$\mathrm{ch}_1(f^*\Upsilon_G) = f^*\mathrm{ch}_1(\Upsilon_G) = f^*\eta ,$$

the upper triangle is commutative. Thus ch_1 is an isomorphism of pointed sets.

Finally, if $\mathrm{Ch}_1(\vartheta) = 0$ then the injectivity of $i_{\mathbb{T}^d}$ implies that $\mathrm{ch}_1(\vartheta) = 0$. Since ch_1 is an isomorphism of pointed sets, ϑ must be the distinguished point in $k_G(X)$, namely the isomorphism class of the trivial $U(m)$-bundle over X. $\square$

3. Application to Schrödinger operators

In this section, we comment on the application of the general results to Schrödinger operators in the form (1). The lattice Γ is represented as

$$\Gamma = \left\{ x \in \mathbb{R}^d : x = \sum_{j=1}^{d} \alpha_j \, \gamma_j \ \text{ for some } \alpha \in \mathbb{Z}^d \right\},$$

where $\{\gamma_1, \ldots, \gamma_d\}$ are independent vectors in $\mathbb{R}^d$. We denote by Γ^* the dual latice of Γ with respect to the standard inner product in $\mathbb{R}^d$, i.e., the lattice generated by the dual basis $\{\gamma_1^*, \ldots, \gamma_d^*\}$ determined through the conditions $\gamma_j^* \cdot \gamma_i = 2\pi\delta_{ij}$, $i, j \in \{1, \ldots, d\}$. The centered fundamental domain Y of Γ is defined by

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

and analogously the centered fundamental domain Y^* of Γ^*. The set Y^* is usually called the *first Brillouin zone* in the physics literature.

3.1. The Bloch–Floquet–Zak representation

As usual in the recent mathematical literature, we use a variant of the Bloch–Floquet transform, which is called the Bloch–Floquet–Zak transform, or just the Zak transform for sake of brevity. The advantage of such a variant is that the fiber at k of the transformed Hamiltonian operator has a domain which does not depend on k.

The Bloch–Floquet–Zak transform is defined as

$$(\mathcal{U}_{\mathrm{Z}}\psi)(k,x) := \sum_{\gamma\in\Gamma} \mathrm{e}^{-\mathrm{i}k\cdot(x+\gamma)}\,\psi(x+\gamma)\,, \quad (k,x)\in\mathbb{R}^{2d}\,, \tag{10}$$

initially for a fast-decreasing function $\psi \in \mathcal{S}(\mathbb{R}^d)$. One directly reads off from (10) the following periodicity properties

$$\big(\mathcal{U}_{\mathrm{Z}}\psi\big)(k,y+\gamma) = \big(\mathcal{U}_{\mathrm{Z}}\psi\big)(k,y) \quad \text{for all} \quad \gamma\in\Gamma\,, \tag{11}$$

$$\big(\mathcal{U}_{\mathrm{Z}}\psi\big)(k+\lambda,y) = \mathrm{e}^{-\mathrm{i}y\cdot\lambda}\,\big(\mathcal{U}_{\mathrm{Z}}\psi\big)(k,y) \quad \text{for all} \quad \lambda\in\Gamma^*\,. \tag{12}$$

From (11) it follows that, for any fixed $k\in\mathbb{R}^d$, $\big(\mathcal{U}_{\mathrm{Z}}\psi\big)(k,\cdot)$ is a Γ-periodic function and can thus be regarded as an element of $\mathcal{H}_{\mathrm{f}} := L^2(T_Y)$, T_Y being the flat torus $\mathbb{R}^d/\Gamma \approx \mathbb{T}^d$.

On the other side, (12) involves a unitary representation of the group of lattice translations on Γ^* (isomorphic to Γ^* and denoted as Λ), given by

$$\tau : \Lambda \to \mathcal{U}(\mathcal{H}_{\mathrm{f}})\,, \quad \lambda\mapsto\tau(\lambda)\,, \quad \big(\tau(\lambda)\varphi\big)(y) = \mathrm{e}^{\mathrm{i}\,y\cdot\lambda}\varphi(y)\,. \tag{13}$$

It is then convenient to introduce the Hilbert space

$$\mathcal{H}_\tau := \Big\{\psi\in L^2_{\mathrm{loc}}(\mathbb{R}^d,\mathcal{H}_{\mathrm{f}}) :\ \psi(k-\lambda) = \tau(\lambda)\,\psi(k) \qquad \forall\lambda\in\Lambda\Big\}\,, \tag{14}$$

equipped with the inner product

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

Obviously, there is a natural isomorphism between $\mathcal{H}_\tau$ and $L^2(Y^*,\mathcal{H}_{\mathrm{f}})$ given by restriction from $\mathbb{R}^d$ to Y^*, and with inverse given by τ-equivariant continuation, as suggested by (12). Equipped with these definitions, one checks that the map defined by (10) extends to a unitary operator

$$\mathcal{U}_{\mathrm{Z}} : L^2(\mathbb{R}^d) \to \mathcal{H}_\tau \cong L^2\big(Y^*, L^2(T_Y)\big)$$

with inverse given by

$$\big(\mathcal{U}_{\mathrm{Z}}^{-1}\varphi\big)(x) = \int_{Y^*} dk\,\mathrm{e}^{\mathrm{i}k\cdot x}\varphi\big(k,[x]\big)\,,$$

where $[\,\cdot\,]$ refers to the a.e. unique decomposition $x=\gamma_x+[x]$, with $\gamma_x\in\Gamma$ and $[x]\in Y$.

As mentioned in the introduction, the advantage of this construction is that the transformed Hamiltonian is a fibered operator over Y^*. Indeed, for the Zak transform of the Hamiltonian operator (1) one finds

$$\mathcal{U}_{\mathrm{Z}}\, H\, \mathcal{U}_{\mathrm{Z}}^{-1} = \int_{Y^*}^{\oplus} dk\, H_{\mathrm{per}}(k)$$

with fiber operator

$$H_{\mathrm{per}}(k) = \frac{1}{2}\big(-\mathrm{i}\nabla_y + k\big)^2 + V_\Gamma(y)\,, \quad k \in Y^*\,. \tag{15}$$

For fixed $k \in Y^*$ the operator $H_{\mathrm{per}}(k)$ acts on $L^2(T_Y)$ with domain[4] $W^{2,2}(T_Y)$ independent of $k \in Y^*$, whenever the potential V_Γ is infinitesimally bounded with respect to $-\Delta$. Under the same assumption on V_Γ, each fiber operator $H(k)$ has pure point spectrum accumulating at infinity: $E_0(k) \leq E_1(k) \leq E_2(k) \leq \dots$

We denote as $\sigma_0(k)$ the set $\{E_i(k) : n \leq i \leq n+m-1\}$, corresponding to a physically relevant family of Bloch bands, and we assume the following *gap condition*:

$$\mathrm{dist}\Big(\sigma_0(k), \sigma\big(H(k)\big) \setminus \sigma_0(k)\Big) \geq g > 0\,, \quad \forall k \in Y^*. \tag{16}$$

Let $P(k) \in \mathcal{B}(\mathcal{H}_{\mathrm{f}})$ be the spectral projector of $H(k)$ corresponding to the set $\sigma_0(k) \subset \mathbb{R}$. The family $\{P(k)\}_{k\in\mathbb{R}^d}$ satisfies assumption (P_1)–(P_3) stated in Section 2. Indeed, the map $k \mapsto P(k)$ is smooth from $\mathbb{R}^d$ to $\mathcal{B}(\mathcal{H}_{\mathrm{f}})$, since $H(k)$ depends smoothly (in the norm-resolvent sense) upon k, and the gap condition (16) holds true. Moreover, from (15) one checks that

$$H(k+\lambda) = \tau(\lambda)^{-1}\, H(k)\, \tau(\lambda)\,, \quad \forall \lambda \in \Lambda\,,$$

and since σ_0 is periodic one concludes that

$$P(k+\lambda) = \tau(\lambda)^{-1}\, P(k)\, \tau(\lambda)\,, \quad \forall \lambda \in \Lambda\,. \tag{17}$$

Property (P_3) corresponds to time-reversal symmetry. This symmetry is realized in $L^2(\mathbb{R}^d)$ by the complex conjugation operator, i.e., by the operator

$$(T\psi)(x) = \bar{\psi}(x)\,, \quad \psi \in L^2(\mathbb{R}^d)\,.$$

By the Zak transform we get that $\tilde{T} = \mathcal{U}_{\mathrm{Z}} T \mathcal{U}_{\mathrm{Z}}^{-1}$ acts as

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

where C is the complex conjugation operator in $\mathcal{H}_{\mathrm{f}}$. Operators in the form (1) commute with the time-reversal operator T. The following statement is analogous to a result proved in [19]. We repeat the proof for the sake of completeness.

Proposition 5 (Time-reversal symmetry). *Assume that the self-adjoint operator H commutes with T in $L^2(\mathbb{R}^d)$, and that $\mathcal{U}_{\mathrm{Z}} H \mathcal{U}_{\mathrm{Z}}^{-1}$ is a* continuously *fibered operator.*

[4]We denote as $W^{k,p}(X)$ the Sobolev space consisting of distributions whose k-th derivative is (identifiable with) an element of $L^p(X)$.

Let $P(k)$ be the eigenprojector of $H(k)$ corresponding to a set $\sigma_0(k)$, satisfying (16). *Then*

$$P(k) = C\,P(-k)\,C\,. \tag{18}$$

Proof. The transformed Hamiltonian $\mathcal{U}_{\mathrm{Z}} H \mathcal{U}_{\mathrm{Z}}^{-1}$ commutes with $\tilde{T}$, yielding a symmetry of the fibers, i.e.,

$$H(k) = CH(-k)C\,. \tag{19}$$

By definition, for any Bloch band E_i one has

$$H(k)\varphi(k) = E_i(k)\varphi(k)$$

for a suitable $\varphi(k) \in \mathcal{H}_{\mathrm{f}}$, $\varphi(k) \neq 0$. By complex conjugation one gets

$$E_i(k)\,C\varphi(k) = CH(k)\varphi(k) = CH(k)C\,C\varphi(k) = H(-k)\,C\varphi(k)\,,$$

which shows that $E_i(k)$ is an eigenvalue of $H(-k)$. By the *continuity* of $k \mapsto E(k,t)$ and the *gap condition*, by starting from $k = 0$ one concludes that $E_i(-k) = E_i(k)$ for any k. Thus $\sigma_0(-k) = \sigma_0(k)$.

Since $P(k) = \chi_{\sigma_0(k)}(H(k))$, where $\chi_{\sigma_0(k)}$ is a smoothed characteristic function whose support contains $\sigma_0(k)$ and no other point of the spectrum of $H(k)$, from (19) one gets (18) by applying the functional calculus and noticing that $f(C\,A\,C) = C\,f(A)\,C$ whenever A is self-adjoint and f is an admissible function. $\square$

We conclude that, in the Zak representation, the family of projectors $\{P(k)\}_{k\in\mathbb{R}^d}$ corresponding to a relevant family of Bloch bands, satisfy assumptions (P_1)–(P_3) of Section 2.

3.2. Comparison with the usual Bloch–Floquet formalism

While from a mathematical viewpoint it is convenient to use the Bloch–Floquet–Zak transform, as defined in (10), in the solid state physics literature one mostly encounters the classical Bloch–Floquet transform, defined by

$$(\mathcal{U}_{\mathrm{B}}\psi)(k,y) := \sum_{\gamma\in\Gamma} e^{-ik\cdot\gamma}\psi(y+\gamma)\,, \quad (k,y)\in\mathbb{R}^{2d} \tag{20}$$

initially for $\psi \in \mathcal{S}(\mathbb{R}^d)$. We devote this short subsection to a comparison of the two choices.

Functions in the range of $\mathcal{U}_{\mathrm{B}}$ are periodic in k and quasi-periodic in y,

$$\big(\mathcal{U}_{\mathrm{B}}\psi\big)(k, y+\gamma) = \mathrm{e}^{\mathrm{i}k\cdot\gamma}\,\big(\mathcal{U}_{\mathrm{B}}\psi\big)(k,y) \quad \text{for all} \quad \gamma\in\Gamma\,, \tag{21}$$

$$\big(\mathcal{U}_{\mathrm{B}}\psi\big)(k+\lambda, y) = \big(\mathcal{U}_{\mathrm{B}}\psi\big)(k,y) \quad \text{for all} \quad \lambda\in\Gamma^*\,. \tag{22}$$

Definition (20) extends to a unitary operator

$$\mathcal{U}_{\mathrm{B}} : L^2(\mathbb{R}^d) \to \mathcal{H}_{\mathrm{B}} := \int_{Y^*}^{\oplus} \mathcal{H}_k\,dk \tag{23}$$

where

$$\mathcal{H}_k := \big\{\varphi \in L^2_{\mathrm{loc}}(\mathbb{R}^d) : \varphi(y+\gamma) = e^{ik\cdot\gamma}\varphi(y) \quad \forall\gamma\in\Gamma\big\}. \tag{24}$$

Although we use the standard (but somehow misleading) "direct integral" notation, it is convenient to keep in mind that the space appearing on the right-hand side is the Hilbert space consisting of the locally-L^2 sections of an Hilbert space bundle with base space Y^* (identified with a d-dimensional torus) and whose fiber at point k is $\mathcal{H}_k$.

The relation between the Bloch–Floquet and the Zak representation is easily obtained by computing the unitary operator $\mathcal{J} = \mathcal{U}_{\mathrm{B}} \mathcal{U}_{\mathrm{Z}}^{-1}$, which is explicitely given by

$$(\mathcal{J}\varphi)(k, y) = \mathrm{e}^{ik\cdot y} \varphi(k, y) .$$

Clearly $\mathcal{J}$ is a fibered operator, whose fiber is denoted as $J(k)$. Notice that $J(k)^{-1}$ maps unitarily the space $\mathcal{H}_k$ into the typical fiber space $\mathcal{H}_0 = \mathcal{H}_{\mathrm{f}} = L^2(T_Y)$. If $H_{\mathrm{B}}(k)$ is the fiber of the Hamiltonian H in Bloch–Floquet representation, one has

$$J(k)\, H_{\mathrm{B}}(k)\, J(k)^{-1} = H_{\mathrm{per}}(k) ,$$

see (15), and thus $\sigma\big(H_{\mathrm{per}}(k)\big) = \sigma\big(H_{\mathrm{B}}(k)\big)$.

As for the relevant family of projectors, we notice that an operator-valued function $k \mapsto P_{\mathrm{B}}(k)$, with $P_{\mathrm{B}}(k) \in \mathcal{B}(\mathcal{H}_k)$, is periodic if and only if $P_{\mathrm{Z}}(k) := J(k)\, P_{\mathrm{B}}(k)\, J(k)^{-1}$ is τ-equivariant with respect to the representation in (13). Moreover, conjugation with $\mathcal{J}$ (resp. with $\mathcal{J}^{-1}$) preserves smoothness and analyticity, since $\mathcal{J}$ acts as a multiplication times a unitary operator $J(k)$ which depends analytically on k. Thus a family of orthogonal projectors $P_{\mathrm{B}}(k)$ is smooth (resp. analytic) and periodic if and only if the corresponding family $P_{\mathrm{Z}}(k)$ is smooth (resp. analytic) and τ-covariant. The results in Section 2 thus directly apply to this situation, yielding the existence of a smooth and periodic orthonormal basis for $\operatorname{Ran} P_{\mathrm{B}}(k)$.

4. Application to Dirac operators

There are experiments in atomic and solid state physics where the relativistic corrections to the dynamics of the electrons are relevant, while the energy scale at which the experiment is performed is not so high to require the use of a fully relativistic theory, namely Quantum Electrodynamics. Such physical situations are conveniently described by using a hybrid model, which embodies some relativistic effects (as, for example, the spin-orbit coupling) without involving the difficulties of a fully relativistic theory.

In order to introduce the model, one first fixes an inertial frame, e.g., the laboratory frame. In such a frame, the potential to which the electron is subject is described by the function $V : \mathbb{R}^d \to \mathbb{R}$. Then it is postulated that the dynamics of the electron in the chosen frame is described by the Dirac equation

$$i\psi_t = H_{\mathrm{D}}\ \psi_t , \quad \psi_t \in L^2(\mathbb{R}^3, \mathbb{C}^4) ,$$

with

$$H_{\mathrm{D}} = -ic\nabla \cdot \alpha + m_{\mathrm{e}} c^2\, \beta + V , \tag{25}$$

where m_{e} denotes the mass of the electron and c the speed of light, and where $\alpha = (\alpha_1, \alpha_2, \alpha_3)$ and β are given by

$$\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix}, \qquad \beta = \begin{pmatrix} 1_{\mathbb{C}^2} & 0 \\ 0 & -1_{\mathbb{C}^2} \end{pmatrix},$$

with $(\sigma_1, \sigma_2, \sigma_3)$ the vector of Pauli spin matrixes.

Such a model is clearly not Lorentz covariant, but it is expected to include the relativistic corrections of lowest order (in the parameter c^{-1}, as $c \to \infty$) to the dynamics described by the Schrödinger equation [24].

We now specialize to the case $V = V_\Gamma$, with V_Γ periodic with respect to a lattice $\Gamma \subset \mathbb{R}^3$. We set $m_{\mathrm{e}} = 1$ and $c = 1$ for simplicity. As in the case of Schrödinger operators, one introduces the Bloch–Floquet–Zak transform, defined as in (10), which yields a unitary operator

$$\mathcal{U}_{\mathrm{Z}} : L^2(\mathbb{R}^3, \mathbb{C}^4) \to L^2(Y^*, \mathcal{H}_{\mathrm{f}}),$$

where $\mathcal{H}_{\mathrm{f}} = L^2(T_Y) \otimes \mathbb{C}^4$ with $T_Y := \mathbb{R}^3/\Gamma$.

The transformed Hamiltonian operator $\mathcal{U}_{\mathrm{Z}} H_{\mathrm{D}} \mathcal{U}_{\mathrm{Z}}^{-1}$ is fibered, with fiber

$$H_{\mathrm{D}}(k) = (-i\nabla + k) \cdot \alpha + \beta + V_\Gamma,$$

acting in $\mathcal{H}_{\mathrm{f}}$, with domain $H^1(T_Y, \mathbb{C}^4)$. Under general assumptions on the periodic potential (e.g., if V_Γ is infinitesimally bounded with respect to $i\nabla$), each fiber $H_{\mathrm{D}}(k)$ has compact resolvent and thus pure point spectrum accumulating to infinity. Since $H_{\mathrm{D}}(k)$ is not bounded from below, the labelling of eigenvalues requires some additional care: one can prove that there is a consistent global labelling $\{\mathcal{E}_n(k)\}_{n\in\mathbb{Z}}$ such that each $k \mapsto \mathcal{E}_n(k)$ is continuous and periodic, and the relation $\mathcal{E}_n(k) \leq \mathcal{E}_{n+1}(k)$ holds true. We say that the function $\mathcal{E}_n$ is the n-th *Bloch–Dirac band*.

Whenever the potential is reflection-symmetric, i.e., $V_\Gamma(-x) = V_\Gamma(x)$, each of the eigenvalues $\mathcal{E}_n(k)$, $n \in \mathbb{Z}$, is at least twofold degenerate, as shown in [14]. Thus, even when considering the projector $P(k)$ corresponding to a single Bloch–Dirac band, one has to deal with the case $m = 2$. This example illustrates the need of the general results stated in Theorem 1 and Theorem 3.

As for time-reversal symmetry, one checks directly that

$$H_{\mathrm{D}}(k)\, T = T\, H_{\mathrm{D}}(-k) \tag{26}$$

where we introduced the antiunitary operator

$$T = -i\,(1 \otimes \alpha_1\alpha_3)\, C,$$

with C denoting complex conjugation in $\mathcal{H}_{\mathrm{f}}$. It is easy to check that $T^2 = 1$ by using the fact that $\alpha_1\alpha_3 = -\alpha_3\alpha_1$.

Let $P(k)$ be the spectral projector of $H_{\mathrm{D}}(k)$ corresponding to a set $\sigma_0(k)$ satisfying (16), and such that $\sigma_0(k+\lambda) = \sigma_0(k)$ for all $\lambda \in \Gamma^*$ and $\sigma_0(-k) = \sigma_0(k)$. As in Section 3, one shows that the map $k \mapsto P(k)$ is smooth and τ-equivariant. Moreover, from (26) and functional calculus it follows that

$$P(-k) = T\, P(k)\, T.$$

Thus the family $\{P(k)\}_{k\in\mathbb{R}^3}$ satisfies Assumptions (P_1), (P_2) and (P_3), and therefore Theorem 1 ensures the triviality of the corresponding complex vector bundle, namely the Bloch–Dirac bundle.

Acknowledgements

I am gratefully indebted with H. Spohn and S. Teufel for suggesting to me to investigate this problem during the preparation of [20], and for many useful discussions. It is a pleasure to thank G. Dell'Antonio, B. Dubrovin, A. Ya. Maltsev for stimulating discussion during the very preliminary phase of this work. Last but not least, I am grateful to R. Percacci for a useful explanation about a result cited in his very recommendable book.

Financial support from DFG and HYKE-project is gratefully acknowledged.

References

[1] S. J. Avis, C. J. Isham, *Quantum field theory and fibre bundles in a general space-time*, in "Recent Developments in Gravitation", eds. M. Lévy and S. Deser, Plenum, (Proceeding of the 1978 NATO Advanced Study Institute, Cargése), 1979.

[2] D. Bleecker, *Gauge theory and variational principles*, Addison-Wesley, 1981.

[3] Ch. Brouder, G. Panati, M. Calandra, Ch. Mourougane, and N. Marzari, *Exponential localization of Wannier functions in insulators*, preprint arXiv cond-mat/0606726 2006.

[4] J. L. Brylinsky, *Loop spaces, characteristic classes and geometric quantization*, Birkhäuser, 1993.

[5] J. des Cloizeaux, *Energy bands and projection operators in a crystal: Analytic and asymptotic properties*, Phys. Rev. **135**, A685–A697, 1964. *Analytical properties of n-dimensional energy bands and Wannier functions*, Phys. Rev. **135**, A698–A707, 1964.

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

[7] K. Fritzsche, H. Grauert, *From holomorphic functions to complex manifolds*, Graduate Text in Mathematics, Springer 2002.

[8] S. Goedecker, *Linear scaling electronic structure methods*, Rev. Mod. Phys. **71**, 1085, 1999.

[9] B. Helffer, J. Sjöstrand, *Équation de Schrödinger avec champ magnétique et équation de Harper*, in *Schrödinger operators* (Sønderborg, August 1988), Lecture Notes in Physics 345, Springer, Berlin, 118–19719, 1989.

[10] D. Husemoller, *Fibre bundles*, Graduate text in Mathematics 20, Springer Verlag, 1966 (2^{nd} edition).

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

[12] A. S. Lyskova, *Topological characteristic of the spectrum of the Schrödinger operator in a magnetic field and in a weak potential*, Theor. Math. Physics, **65**, no. 3, 1218–1225, 1985.

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

[14] U. Mauthner, *The Dirac equation with periodic potential.* Ph. D. Thesis, Technische Universität München, in preparation.

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

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

[17] G. Nenciu, *Existence of the exponentially localised Wannier functions*, Comm. Math. Phys. **91**, no. 1, 81–85, 1983.

[18] S. P. Novikov, *Magnetic Bloch functions and vector bundles. Typical dispersion law and quantum numbers*, Sov. Math. Dokl. **23**, no. 2, 298–303, 1981.

[19] G. Panati, Ch. Sparber, and S. Teufel, *Geometric currents in piezoelectricity*, preprint arXiv math-ph/0606044, 2006.

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

[21] R. Percacci, *Geometry of nonlinear field theories*, World Scientific, 1986.

[22] E. H. Spanier, *Algebraic topology*, McGraw-Hill, 1966.

[23] N. Steenrod, *The Topology of fibre bundles*, Princeton University Press, 1951.

[24] B. Thaller, *The Dirac equation*, Texts and Monographs in Physics, SpringerVerlag, 1992.

[25] D. J. Thouless, *Wannier functions for magnetic sub-bands*, J. Phys. C: Solid State Phys. **17**, L325–L327, 1984.

[26] A. Weil, *Variétés Kaehlériennes*, Hermann, 1957.

Gianluca Panati
Zentrum Mathematik and Physik Department
Technische Universität München
D-80290 München
Germany
e-mail: `panati@mat.uniroma1.it`

Communicated by Vincent Rivasseau.

Submitted: October 5, 2006.

Accepted: November 11, 2006.