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On the localization dichotomy for gapped quantum systems

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To Eloisa

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Introduction

*All the bases are equal, but some
bases are more equal than others.*

The issue of choosing the right reference frame or the right basis is crucial in physics and mathematics. As it is taught in any basic course of linear algebra, given a diagonalizable linear transformation on a finite dimensional vector space, one can choose, amongst the infinite number of bases of the vector space, a basis that better describes the linear transformation, namely a basis that diagonalizes the transformation. In general the situation is more complicated and the choice of a proper basis depends on the peculiarities of the problem we are interested in.

A clear example of this basis issue can be found in the study of solid state physics. In the independent particle approximation, the one particle Schrödinger operator that describes a crystalline insulating system usually has an absolutely continuous spectrum. This means that the set of occupied states of the system corresponds to an infinite dimensional subspace of the Hilbert space, corresponding to the pure states of the system. Therefore it is necessary to choose a particular basis for the subspace in order to make explicit computations. A special basis for this type of problem has been introduced by G. Wannier in 1937 [113], the so called *Wannier basis*. This basis clearly reflects the translational symmetry of the problem and, due to its ladder structure, is easy to handle. Nowadays Wannier functions are extensively used in computational physics to represent the charge distribution in crystalline solids [75]. Shortly, we can say that Wannier functions are to crystalline solids what atomic orbitals are to isolated atoms. The spreading of the use of Wannier basis in the scientific community has a twofold explanations: on one hand, the Wannier functions turned out to be a very efficient tool for computational problems [74], since their use has the advantage to reduce the computational time to a linear growth with respect to the size of the sample (in contrast to old methods that show a cubic dependence on the sample size) [55]; on the other hand, they provide a theoretical framework able to describe phenomena where the behaviour of the electrons can be described by semiclassical approaches, for example in the piezoelectric effect [100]. The problem of a rigorous mathematical proof of the existence of exponentially localized Wannier functions for time-reversal symmetric systems traces back to the work of W. Kohn [67], with remarkable contributions by G. Nenciu [84, 86], B. Helffer and J. Sjöstrand [61] and by the Italian group [89, 20, 90, 47].

In the last decades, starting with the discovery of the Quantum Hall effect by

K. von Klitzing in 1981, the interest in insulating materials has seen an incredible boost, see [25]. In fact, the two-dimensional Quantum Hall system is now recognized as the archetypical example of what is called a *topological insulator*: a particular material that is insulating in the bulk but can sustain a current on its edge [56]. The discovery of these peculiar systems required the development of new mathematical techniques being able to catch their exotic character.

The Wannier basis is commonly used to study the bulk properties of the physical systems under consideration. Therefore, it is legitimate to ask if this special basis is suitable for the study of topological insulators, in particular whether it is able to discern if a specific system is a topological insulator or not. A first step in this direction has been made by D.J. Thouless, in 1984 [111]. In his paper Thouless showed that, for the Landau Hamiltonian, the projection onto a single Landau level cannot admit a basis of *well localized* Wannier functions. In this context well localized functions means functions whose tails decay at least as $\|\mathbf{x}\|^{-2}$, as $\|\mathbf{x}\| \rightarrow \infty$. This fact admits an intuitive physical explanation: the slow decaying of the Wannier functions implies an infinite second moment of the probability measure associated to the Wannier function. This delocalization is interpreted in [79] as a reflection of the quantized bulk current that flows in the sample. Nevertheless, the mathematical justification of Thouless' argument for general Hamiltonian comes only in 2016, when the existence of a critical exponent for the tails of the Wannier functions and its relation to quantum transport has been rigorously proven by Monaco, Panati, Pisante and Teufel [79] in the context of periodic gapped quantum systems. In particular, they showed that the optimally localized Wannier functions for an isolated group of energy bands can have only two possible types of tails decay, depending on the topology of the bands under considerations: either they are exponentially decaying or polynomially decaying with exponent $\alpha > -2$ in dimension $d = 2$. This result has been dubbed *localization dichotomy* in [79].

Although the results in [79] provides a complete and satisfying picture in the case of periodic systems, it is a fact of life that perfect crystalline systems do not exist in nature. Hence, the topological property of the systems must not depend on the translational symmetry of the model. In this thesis, we foster the concept of generalized Wannier basis as a suitable tool to understand the topological properties of disordered systems. The generalized Wannier basis has been mathematically studied for the first time in two significant works by A. Nenciu and G. Nenciu [82, 83]. In particular, the long term goal of this work is to extend the localization dichotomy to disordered systems. In the following pages we present the state of art of the theory, we state a precise mathematical conjecture on the problem and report about the original results achieved.

The localization dichotomy for periodic gapped quantum systems lays its basis on two fundamental pillars: the well posed definition of Wannier functions on the one hand and the characterization of the Bloch bundle by means of the Chern number on the other hand. It is the intertwining of this two concepts that leads to the proof of the localization dichotomy. Therefore, it is important to understand how these two objects can be extended to a non periodic framework. The first three chapters of the thesis are devoted exactly to this scope. In particular:

1. in Chapter 1 we review the theory of Wannier functions (WF) and their

generalization for non periodic systems, the so called generalized Wannier functions.

2. Chapter 2 is dedicated to the understanding of what happens to the Chern number when translation symmetry is broken and the Bloch bundle cannot be constructed. Firstly we define the Chern character by means of the magnetic Bloch–Floquet transformation. Then, filling some missing details in the literature, we prove the Středa formula for continuous periodic gapped quantum systems. In the end we study the Chern character through the magnetic field response of the integrated density of states. In the literature this relation goes under the name of gap labelling theorem. In particular we provide a new proof of the gap labelling theorem and we extend it, in an approximate sense, to the case of slowly varying magnetic field.
3. In Chapter 3 we study in detail an example of Wannier-like functions for disordered systems in any dimension, namely the Prodan’s radial Wannier functions. We prove the existence of this generalized basis also for non trivial topological bands and investigate its relations with the transport properties of the physical system.

After having settled the necessary basis for understanding the localization dichotomy in a non periodic setting, in Chapter 4 we state the conjecture on the localization dichotomy for gapped quantum systems and we prove that the existence of a generalized Wannier basis in the sense of Chapter 1 implies that the Chern character is equal to zero.

Eventually, in Chapter 5 we investigate what happens when the definition of Wannier basis is modified. Specifically, we drop the linear independence condition in the definition of the Bloch frame, defining the so called Parseval frames. For topological trivial bands we provide an explicit construction of the exponentially localized Wannier basis, instead for topological non trivial bands we provide an explicit construction of the exponentially localized Parseval frame. We extend the proof by continuity of generalized Wannier basis/frame to the case of constant magnetic field perturbation, admitting irrational value of the magnetic flux.

Since the materials contained in the thesis are the fruits of joint collaborations with different people, despite our efforts to use a coherent notation in the whole thesis, we could guarantee coherence and consistency of notation only chapter-wise.

All the chapters except the first one contain original material:

- Part of Chapter 2, whose principal results are Theorem 2.4.1 and Theorem 2.4.5, is the fruit of a joint collaboration with H. Cornean and D. Monaco and it has been submitted to a scientific journal for publication, the preprint can be found on arXiv <https://arxiv.org/pdf/1810.05623> [32].
- The material in Chapter 3 is based on a joint work with G. Panati. Theorem 3.1.1 and Proposition 3.2.4 describe the original results. The final manuscript is in preparation.

- In Chapter 4, Theorem 4.2.1 is the main result and it is the fruit of a joint collaboration with G. Marcelli and G. Panati; the corresponding manuscript is soon to be completed.
- Chapter 5 can be found on arXiv <https://arxiv.org/pdf/1704.00932> [33] and the main contributions of the author regard Section 5.2, Section 5.4, Section 5.8 and Section 5.9. The main results are summarized in Theorem 5.3.4, Theorem 5.4.1 and Corollary 5.4.3. The paper is the result of a joint work with H. Cornean and D. Monaco and it has been accepted for publication in *Communication in Mathematical Physics*.

The interplay between physics and mathematics found a fertile ground in the exotic phenomena of solid state physics and the understanding of physical phenomena by means of Wannier functions is an example of this fruitful interaction. We hope that the results presented hereafter could make a small contribution to the improvement of this framework and be the starting point for further future developments.

Chapter 1

Generalized Wannier functions

In this first chapter we start by recalling the definition and fundamental properties of the Wannier functions for periodic systems, then we review the different definitions of Wannier functions for non periodic systems, namely the *generalized Wannier functions*.

1.1 Heuristic physical picture

The mathematical foundations of the physics of condensed matter systems stands on the (non relativistic) many-body theory of quantum mechanics, in which the role of the leading actor is played by the many body Schrödinger equation. A complete physical and mathematical model of a sample of material requires to take into account the quantum dynamics of the nuclei and the electrons, considering their quantum statistical nature and their mutual interaction mediated by the Coulomb interaction. Nevertheless, considering that in a small sample of material the number of “quantum bodies”, which is the sum of N electrons and M nuclei, is usually of the order of magnitude of $10^{24} \sim 10^{27}$, finding an exact solution to the many body Schrödinger equation is a very challenging task, if not virtually impossible.

Therefore, this impasse is usually overcome by making approximations that are physically and (not always) mathematically consistent and justified [24]. As a first approximation, one can neglect the effect of the spin on the dynamics and, at a non relativistic energy scale regime, the dynamics of the electrons and the nuclei can be decoupled. Indeed, in view of the mass difference between electrons and nuclei, one can assume that the nuclei are governed by a classical dynamics, whereas the electrons are described using the law of quantum mechanics. This is the well-known Born-Oppenheimer approximation, and there is a vast literature about it, both at the physical and mathematical level. As a further approximation, one can assume that the nuclei are fixed, hence their coordinates become parameters on which the state of the system depends on. This approximation is quite rude and exclude a priori the description of interesting physical phenomena in which the role of the motion of the nuclei is important, for example the phonons interactions.

In the end, the resulting Hamiltonian operators describes only the degrees of freedom of the electrons. The essential information that one would like to extract from a model of a physical system, is the value of its ground state, namely the

minimum of its energy. Despite of the approximations made, it remains very difficult to prove the existence of the ground states for the electronic many body Schrödinger operator, especially since one is interested in the *thermodynamics limit* of the system, that amounts to assume the sample to be infinite and with an infinite number of electrons, but with finite number of electrons per unit volume (note that in this case the aim is to find the minimum of the energy per unit volume). Since the dawn of quantum mechanics this has been a very active research field, and there is a vast literature on the subject. Without entering in the delicate details of the problem, we mention that a fruitful strategy turned out to be the Hartree-Fock theory. The basic idea is to minimize the energy of the system only on a specific set of configurations. Whenever the minimizer exists, it is called ground state of the system. Using the Hartree-Fock approach, recently it has been proven [22] that for a crystal with some defects, the ground state of the system is given exactly by the projection on a spectral subspace of a one body Schrödinger operator. As a product of the minimization procedure, the one body Hamiltonian operator encapsulates the information of the interactions between the electrons and between the nuclei and the electrons.

In this sense, the one body Hamiltonian operators that appear in this thesis has to be thought as “mean field” operators, which contains, even though in an approximate way, the information about the whole interacting many body physical system.

1.2 Periodic case

Let us start by reviewing the model of a perfect crystal at zero temperature. Consider the Hilbert space $L^2(\mathbb{R}^d)$ with $d \leq 3$ and a regular lattice Γ in \mathbb{R}^d , that is

$$\Gamma = \left\{ \mathbf{x} \in \mathbb{R}^d \mid \mathbf{x} = \sum_{i=1}^d a_i \mathbf{b}_i, a_i \in \mathbb{Z} \right\} \subset \mathbb{R}^d,$$

where the d vectors \mathbf{b}_i , $1 \leq i \leq d$, called the generators of the lattice, are chosen to be of norm one. Then consider the Hamiltonian ¹

$$H_\Gamma = \frac{1}{2} (\mathbf{P} - \mathbf{A}_\Gamma)^2 + V_\Gamma \quad (1.2.1)$$

where \mathbf{P} is the momentum operator, that is the differential operator of first order given by

$$\mathbf{P} := -i\nabla = -i(\partial_1, \dots, \partial_d),$$

$\mathbf{A}_\Gamma = (A_{\Gamma,1}, \dots, A_{\Gamma,d})$ is the vector of multiplication operators that is associated to the magnetic vector potential and V_Γ is the multiplication operator associated to the scalar electrostatic potential. Both \mathbf{A}_Γ and V_Γ are supposed to be Γ -periodic, namely

$$\mathbf{A}_\Gamma(\mathbf{x} + \gamma) = \mathbf{A}_\Gamma(\mathbf{x}), \quad V_\Gamma(\mathbf{x} + \gamma) = V_\Gamma(\mathbf{x}), \quad \forall \mathbf{x} \in \mathbb{R}^d, \gamma \in \Gamma.$$

¹We use the Hartree unit system $\hbar = 1 = e = m_e$.

In order to not obscure the key points of the theory, we assume that $\mathbf{A}_\Gamma \in C^\infty(\mathbb{R}^d, \mathbb{R}^d)$ and $V_\Gamma \in C^\infty(\mathbb{R}^d)$ are uniformly bounded with all their derivatives. In Remark 1.2.5 we discuss the generalization of the theory to unbounded and less regular potentials. Under these assumptions, the domain of the Hamiltonian coincides with the Sobolev space $H^2(\mathbb{R}^d)$.

Define, for every $\gamma \in \Gamma$, the set of unitary operators $\{T_\gamma\}_{\gamma \in \Gamma}$, where

$$(T_\gamma f)(\mathbf{x}) = f(\mathbf{x} - \gamma),$$

namely the operator associated with a translation by a vector $\gamma \in \mathbb{R}^d$. A straightforward computation shows that

$$\begin{aligned} T_\gamma T_\eta &= T_{\gamma+\eta}, & \forall \gamma, \eta \in \Gamma, \\ T_\gamma^* &= T_\gamma^{-1} = T_{-\gamma}. \end{aligned}$$

This implies that the set $\{T_\gamma\}_{\gamma \in \Gamma}$ is a unitary representation of the discrete group $\mathbb{Z}^d \simeq \Gamma$. That is, there exists a group homomorphism $T_\bullet : \mathbb{Z}^d \rightarrow \mathfrak{U}(\mathcal{H})$, where $\mathfrak{U}(\mathcal{H})$ denotes the subset of unitary operators in $\mathcal{B}(\mathcal{H})$. By direct computation one can show that

$$HT_\gamma = HT_\gamma$$

for all $\gamma \in \Gamma$. This is the mathematical footprint of the fact that the Schrödinger equation is modelling a translation invariant system and that \mathbb{Z}^d is a symmetry group for the physical system [115]. Due to the underlying periodic structure it is useful to imagine the whole space as being the union of small cells. Indeed, one can decompose \mathbb{R}^d in a disjoint sum of unit cells Ω centred at the points of the lattice Γ , that is

$$\Omega := \left\{ \mathbf{x} \in \mathbb{R}^d \mid \mathbf{x} = \sum_{i=1}^d a_i \mathbf{b}_i, a_i \in \left(-\frac{1}{2}, \frac{1}{2}\right] \right\},$$

and $\mathbb{R}^d = \bigsqcup_{\gamma \in \Gamma} (\Omega + \gamma)$. We then introduce the concept of dual lattice. The dual lattice Γ^* of Γ is given by the set

$$\Gamma^* := \left\{ \mathbf{x} \in \mathbb{R}^d \mid \mathbf{x} \cdot \gamma \in 2\pi\mathbb{Z}, \forall \gamma \in \Gamma \right\},$$

where we identify the generators of the dual lattice as \mathbf{d}_i , $i = 1, \dots, d$. Accordingly one defines the unit cell of the dual lattice, which in the physical literature is known as Brillouin zone, by

$$\mathbb{B} := \left\{ \mathbf{x} \in \mathbb{R}^d \mid \mathbf{x} = \sum_{i=1}^d c_i \mathbf{d}_i, c_i \in \left(\frac{1}{2}, \frac{1}{2}\right] \right\}.$$

Therefore, in order to properly study the properties of the system one needs a tool that is capable to grasp the periodicity of the problem and the induced separation of scales: the microscopic scale of the unit cell and the macroscopic scale of the crystal as a whole. The right tool for this task is given by the Bloch–Floquet–Zak unitary transform. Consider a vector $\psi \in C_0^\infty(\mathbb{R}^d) \subset L^2(\mathbb{R}^d)$ and define

$$(\mathcal{U}_{\mathcal{BFZ}}\psi)(\mathbf{k}, y) = \frac{1}{|\mathbb{B}|^{1/2}} \sum_{\gamma \in \Gamma} e^{-i\mathbf{k} \cdot (y - \gamma)} \psi(y - \gamma), \quad \mathbf{k} \in \mathbb{R}^d, y \in \mathbb{R}^d. \quad (1.2.2)$$

where $|\mathbb{B}|$ denotes the volume of the Brillouin zone. We note that the compactness support property of $C_0^\infty(\mathbb{R}^d)$ guarantees that the transform $\mathcal{U}_{\mathcal{BFZ}}$ is a well defined operator. Moreover we observe that it satisfies the following relations

$$\begin{aligned} (\mathcal{U}_{\mathcal{BFZ}}\psi)(\mathbf{k}, y + \gamma) &= (\mathcal{U}_{\mathcal{BFZ}}\psi)(\mathbf{k}, y), \quad \forall \gamma \in \Gamma, \\ (\mathcal{U}_{\mathcal{BFZ}}\psi)(\mathbf{k} + \gamma^*, y) &= e^{-i\gamma^* \cdot y} (\mathcal{U}_{\mathcal{BFZ}}\psi)(\mathbf{k}, y), \quad \forall \gamma^* \in \Gamma^*. \end{aligned}$$

Because of that we say that $\mathcal{U}_{\mathcal{BFZ}}\psi$ is Γ^* -pseudo-periodic in the first variable and Γ -periodic in the second variable. Consider now the unit cell Ω endowed with periodic boundary conditions, that is $\mathbb{T}^d := \mathbb{R}^d/\Gamma$. Following [92], a more elegant way to describe pseudo-periodicity requires the introduction of the operators $(\tau(\gamma^*)f)(y) = e^{-i\gamma^* \cdot y} f(y)$, for all $f \in L^2(\mathbb{T}^d)$. An easy computation shows that $\tau(\cdot) : \Gamma^* \rightarrow \mathfrak{U}(L^2(\mathbb{T}^d))$ is a unitary representation of the set Γ^* , which as a discrete group is isomorphic to \mathbb{Z}^d . Therefore it is convenient to define the space

$$\mathcal{H}_\tau := \left\{ \psi \in L_{loc}^2(\mathbb{R}^d, L^2(\mathbb{T}^d)) \mid \psi(\mathbf{k} + \gamma^*) = \tau(\gamma^*)\psi(\mathbf{k}), \forall \gamma^* \in \Gamma^* \right\}.$$

The space \mathcal{H}_τ is, up to an isomorphism, an example of direct integral of Hilbert spaces, namely

$$\mathcal{H}_\tau \simeq \int_{\mathbb{B}}^\oplus d\mathbf{k} L^2(\mathbb{T}^d),$$

see [98, Section XIII.16] for a precise definition of the notation. In particular, it is a Hilbert space endowed with the sesquilinear form defined by

$$\langle \psi, \varphi \rangle_{\mathcal{H}_\tau} = \int_{\mathbb{B}}^\oplus d\mathbf{k} \langle \psi(\mathbf{k}), \varphi(\mathbf{k}) \rangle_{L^2(\mathbb{T}^d)}.$$

Then we have the following results:

Proposition 1.2.1 (Bloch–Floquet–Zak transform, [92]). *The Bloch–Floquet–Zak transform is a unitary Hilbert space isomorphism between $L^2(\mathbb{R}^d)$ and \mathcal{H}_τ ,*

$$\mathcal{U}_{\mathcal{BFZ}} : L^2(\mathbb{R}^d) \rightarrow \mathcal{H}_\tau.$$

Since H_Γ commutes with the set of unitary operators $\{T_\gamma\}_{\gamma \in \Gamma}$, we obtain a fibered Hamiltonian [98, Section XIII.16] :

$$\mathcal{U}_{\mathcal{BFZ}} H_\Gamma \mathcal{U}_{\mathcal{BFZ}}^* = \int_{\mathbb{B}}^\oplus d\mathbf{k} h(\mathbf{k}) \tag{1.2.3}$$

where $h(\mathbf{k})$ is Γ^* covariant in the sense that

$$h(\mathbf{k} + \gamma^*) = \tau^*(\gamma^*) h(\mathbf{k}) \tau(\gamma^*), \quad \forall \gamma^* \in \Gamma^*.$$

This implies that whenever two fiber Hamiltonians $h(\mathbf{k})$ differ by a dual lattice vector they are unitarily equivalent. Because of that, the spectral properties of the family $\{h(\mathbf{k})\}_{\mathbf{k} \in \mathbb{R}^d}$ can be completely recovered from the subfamily $\{h(\mathbf{k})\}_{\mathbf{k} \in \mathbb{B}}$.

Let us now look more carefully at the operator $h(\mathbf{k})$. The fiber Hamiltonian $h(\mathbf{k})$ is given by

$$h(\mathbf{k}) := \frac{1}{2} (-i\nabla_y - \mathbf{A}_\Gamma(y) - \mathbf{k})^2 + V_\Gamma(y)$$

where we have denoted by $-i\nabla_y$ the gradient that acts on $L^2(\mathbb{T}^d)$, i. e. with periodic boundary conditions, and with a little abuse of notation we have denoted by $V_\Gamma(y)$ and $\mathbf{A}_\Gamma(y)$ the multiplication operators on $L^2(\mathbb{T}^d)$ associated to V_Γ and \mathbf{A}_Γ . Note that, due to the regularity of the potentials, the domain of $h(\mathbf{k})$ is independent of \mathbf{k} and it is given by the Sobolev space $H^2(\mathbb{T}^d)$. Expanding the square we obtain that

$$h(\mathbf{k}) = -\frac{1}{2}\Delta_y + \mathbf{k} \cdot \mathbf{W} + W_0,$$

where $\mathbf{W} = (W_1, \dots, W_d)$ and W_0 are infinitesimally bounded (or “Kato small”) operators with respect to the Laplacian. Then, applying [98, Lemma 16] we obtain that $h(\mathbf{k})$ is an entire family in the sense of Kato². Using standard results in perturbation theory and the fact that $-\Delta_y$ has discrete spectrum that accumulates only at infinity, it follows that $h(\mathbf{k})$ has a discrete spectrum for every $\mathbf{k} \in \mathbb{C}^d$. Now we focus the attention only at $\mathbf{k} \in \mathbb{B}$. The analyticity property of the function $\mathbb{B} \ni \mathbf{k} \rightarrow h(\mathbf{k})$ implies that the spectrum of $h(\mathbf{k})$ “changes smoothly” with respect to \mathbf{k} . Let us summarize all these results in the next theorem.

Theorem 1.2.2 (Properties of $h(\mathbf{k})$, [98, 71]). *Consider the family $\{h(\mathbf{k})\}_{\mathbb{R}^d}$ defined before, then:*

(i) *The family $\{h(\mathbf{k})\}_{\mathbb{R}^d}$ is an entire analytic family in the sense of Kato with compact resolvent.*

(ii) *The spectrum of each $h(\mathbf{k})$ is discrete. The eigenvalues are labelled increasingly by*

$$\lambda_1(\mathbf{k}) \leq \lambda_2(\mathbf{k}) \leq \dots \lambda_i(\mathbf{k}) \leq \dots, \quad i \in \mathbb{N}.$$

(iii) *The functions $\mathbb{R}^d \ni \mathbf{k} \mapsto \lambda_i(\mathbf{k})$ are Γ -periodic, continuous and piecewise analytic.*

(iv) *The spectrum of H_Γ can be reconstructed from the spectrum of the family $\{h(\mathbf{k})\}_{\mathbf{k} \in \mathbb{B}}$, namely*

$$\sigma(H) = \bigcup_{\mathbf{k} \in \mathbb{R}^d} \sigma(h(\mathbf{k})) = \{E \in \mathbb{R} \mid \exists i \in \mathbb{N}, \mathbf{k} \in \mathbb{B} \text{ s.t. } \lambda_i(\mathbf{k}) = E\}.$$

(v) *In absence of locally flat bands, that is $\lambda_j(\mathbf{k}) = E$ for all $\mathbf{k} \in M$ with $|M| > 0$, the spectrum of H_Γ is purely absolutely continuous.*

Note that the set $\Sigma := \{(\mathbf{k}, \lambda) \in \mathbb{B} \times \mathbb{R} \mid \lambda \in \sigma(h(\mathbf{k}))\}$, that is sometimes called Bloch variety, is an analytic manifold [51, 71] and it is the rigorous mathematical definition of what is called *energy band picture* in the physics literature. Borrowing the same terminology we usually refer to the graph of $\mathbb{B} \ni \mathbf{k} \mapsto \lambda_i(\mathbf{k})$ as to the i -th (*energy or Bloch*) *band*.

Throughout all this thesis, a crucial role will be played by spectral gapped Hamiltonians. When we talk about general gapped systems we mean that the Hamiltonian governing the dynamics of the system has a spectral island, namely there exists a part of the spectrum that is isolated from the rest.

²The family of operators $\{h(\mathbf{k})\}_{\mathbb{R}^d}$ is such that the domain of $h(\mathbf{k})$ is a set $\mathcal{D}(h(\mathbf{k})) := H^2(\mathbb{T}^d)$ independent on $\mathbf{k} \in \mathbb{R}^d$ and, for every $\varphi \in \mathcal{D}(h(\mathbf{k}))$, the vector valued function $h(\mathbf{k})\varphi$ is analytic in \mathbf{k} [98, p.16].

Assumption 1.2.3 (Spectral gap assumption). We say that the Hamiltonian H_Γ satisfies a spectral gap assumption if it has a spectral island σ_0 isolated from the rest of the spectrum, that is there exists $g > 0$ such that

$$\text{dist}(\sigma_0, \sigma(H) \setminus \sigma_0) = g. \quad (1.2.4)$$

Notice that in the context of periodic Schrödinger operators the notion of spectral gap can be relaxed allowing the presence of local gaps only. Let us be more precise.

Assumption 1.2.4 (Local gap assumption). We say that the Hamiltonian H_Γ satisfies a local gap assumption if there exists a group of m bands such that they are isolated from the other part of the spectrum, that is, define $\sigma_0(\mathbf{k}) = \{\lambda_i(\mathbf{k}), j \leq i \leq j + m, i, j \in \mathbb{N}\}$, then there exists $g > 0$ such that

$$\inf_{\mathbf{k} \in \mathbb{B}} \text{dist}(\sigma_0(\mathbf{k}), \sigma(h(\mathbf{k})) \setminus \sigma_0(\mathbf{k})) = g.$$

Clearly, a Hamiltonian satisfying the local gap conditions satisfies also the spectral gap condition.

Remark 1.2.5. As we have mentioned before, all the results regarding the fibered Hamiltonian can be extended to unbounded vector and scalar potentials \mathbf{A}_Γ and V_Γ . As soon as the family $\{h(\mathbf{k})\}_{\mathbf{k} \in \mathbb{B}}$ is an analytic family in the sense of Kato with compact resolvent, all the results of the previous section holds. For example, it is enough to require that $\mathbf{A}_\Gamma \in L^\infty(\mathbb{T}^2, \mathbb{R}^2)$ when $d = 2$ or $\mathbf{A}_\Gamma \in L^4(\mathbb{T}^3, \mathbb{R}^3)$ when $d = 3$ and $\nabla \cdot \mathbf{A}_\Gamma, V_\Gamma \in L^2_{\text{loc}}(\mathbb{R}^d)$ when $2 \leq d \leq 3$. Others examples regarding weaker hypothesis on the potentials can be found in [79, Remark 3.2] and references therein.

1.2.1 Wannier functions and composite Wannier functions

Assume now that the Hamiltonian H_Γ satisfies the spectral gap Assumption 1.2.3. By means of the Riesz formula we can define the projection P_0 onto the spectral island σ_0

$$P_0 := \frac{i}{2\pi} \oint_{\mathcal{C}} dz (H_\Gamma - z)^{-1},$$

where \mathcal{C} is a positively oriented contour encircling σ_0 . We are now interested in finding an orthonormal basis of the range of P_0 . The results of the previous section implies that P_0 can be fibered via the Bloch–Floquet–Zak transformation, namely

$$P_0 = \int_{\mathbb{B}}^{\oplus} d\mathbf{k} P_0(\mathbf{k}), \quad P_0(\mathbf{k}) = \frac{i}{2\pi} \oint_{\mathcal{C}(\mathbf{k})} dz (h(\mathbf{k}) - z)^{-1}.$$

The main features of the family of projections $\{P_0(\mathbf{k})\}_{\mathbf{k} \in \mathbb{R}^d}$ are collected in the following proposition.

Proposition 1.2.6 ([90] and references therein). *The family of projections $\{P_0(\mathbf{k})\}_{\mathbf{k} \in \mathbb{R}^d}$ satisfies the following properties.*

- (i) *The map $\mathbf{k} \mapsto P_0(\mathbf{k})$ is a smooth map from \mathbb{R}^d to $\mathcal{B}(L^2(\mathbb{T}^d))$, where $\mathcal{B}(L^2(\mathbb{T}^d))$ is equipped with the operator norm.*

(ii) The map $\mathbf{k} \mapsto P_0(\mathbf{k})$ extends to an analytic $\mathcal{B}(L^2(\mathbb{T}^d))$ -valued function on the domain

$$S_\alpha := \{\mathbf{k} \in \mathbb{C}^d \mid |\operatorname{Im}(\mathbf{k})| < \alpha\} \quad (1.2.5)$$

for some $\alpha > 0$.

(iii) The map $\mathbf{k} \mapsto P_*(\mathbf{k})$ is τ -covariant, that is

$$P_0(\mathbf{k} + \gamma^*) = \tau^*(\gamma^*)P_0(\mathbf{k})\tau(\gamma^*), \quad \forall \gamma^* \in \Gamma^*.$$

Remark 1.2.7. The proof of Proposition 1.2.6 is based on the analyticity properties of the family $\{h(\mathbf{k})\}_{\mathbf{k} \in \mathbb{R}^d}$ and on Assumption 1.2.3. Note that for these results it is sufficient for the Hamiltonian to satisfy a local gap condition, namely Assumption 1.2.4. Then, despite the fact that P_0 is ill defined, the family $\{P_0(\mathbf{k})\}_{\mathbf{k} \in \mathbb{R}^d}$ is well defined because it is possible to find a contour $\mathcal{C}(\mathbf{k})$ for every $\mathbf{k} \in \mathbb{R}^d$. Moreover, the local gap assumption assures that the contour can be chosen locally constant with respect to \mathbf{k} , see [90] for more details.

Consider now for simplicity the case of $\dim(\operatorname{Rank} P_0(\mathbf{k})) = 1$, that is $\sigma_0(\mathbf{k}) = \{\lambda_j(\mathbf{k})\}$ for a specific $j \in \mathbb{N}$. This means that an orthonormal basis for the range of $P_0(\mathbf{k})$ is simply given by a normalized solution to

$$h(\mathbf{k})\varphi_j(\mathbf{k}) = \lambda_j(\mathbf{k})\varphi_j(\mathbf{k}). \quad (1.2.6)$$

A normalized solution $\varphi_j(\mathbf{k})$ is called *Bloch function*. Recalling the idea of atomic orbital for the single atoms, a Bloch function can be thought as \mathbf{k} -space analogue of an atomic orbital for an infinite lattice of atoms. Note that for periodic systems the spectrum of the Hamiltonian is usually absolutely continuous, therefore it is not possible to have proper atomic orbitals, namely square integrable eigenfunctions of the Hamiltonian. Consider now the inverse Bloch–Floquet–Zak transform of the Bloch function, namely

$$\psi_0(\mathbf{x}) := (\mathcal{U}_{\mathcal{BFZ}}^{-1}\varphi_j)(\gamma + \underline{x}) := \frac{1}{|\mathbb{B}|^{1/2}} \int_{\mathbb{B}} d\mathbf{k} e^{i\mathbf{k} \cdot (\gamma + \underline{x})} \varphi_j(\mathbf{k}, \underline{x}), \quad (1.2.7)$$

where we have used the unique decomposition of every point $\mathbf{x} \in \mathbb{R}^d$ as

$$\mathbf{x} = \gamma + \underline{x}, \quad \gamma \in \Gamma, \quad \underline{x} \in \Omega.$$

The function ψ is called *Wannier function*. It is the real space counterpart of the Bloch functions and it is analogous to a crystalline atomic orbital. Consider now the translation operator T_γ and

$$w_\gamma(\mathbf{x}) := (T_\gamma\psi_0)(\mathbf{x}) = \frac{1}{|\mathbb{B}|^{1/2}} \int_{\mathbb{B}} d\mathbf{k} e^{i\mathbf{k} \cdot (\mathbf{x} - \gamma)} \varphi_j(\mathbf{k}, \underline{x}). \quad (1.2.8)$$

From the properties of the Bloch–Floquet–Zak transform it is not difficult to prove that the set

$$\{T_\gamma\psi_0\}_{\gamma \in \Gamma}$$

is an orthonormal basis for the range of P_0 . The importance of the Wannier functions relies on their localization properties. In particular their spatial localization is tightly

correlated to the regularity of the Bloch functions with respect to \mathbf{k} . In view of the similarity of $\mathcal{U}_{\mathcal{BFZ}}$ with the Fourier transform, this relation is not surprising, it is exactly the analogue of the integrability-regularity relation that holds true in harmonic analysis.

The relation between regularity of Bloch functions and spatial localization of Wannier functions is summarized in the following proposition, where in order to simplify the notation, we use the Japanese bracket notation. Let $\mathbb{R}^d \ni \mathbf{x} = (x_1, \dots, x_d)$, then

$$\langle \mathbf{x} \rangle := \left(1 + \|\mathbf{x}\|^2\right)^{\frac{1}{2}}$$

is called the Japanese bracket of \mathbf{x} .

Proposition 1.2.8. *Consider $\mathcal{U}_{\mathcal{BFZ}} : L^2(\mathbb{R}^d) \rightarrow \mathcal{H}_\tau$. Then, for every $s \in \mathbb{N}$,*

- (i) $\langle \mathbf{x} \rangle^s \psi \in L^2(\mathbb{R}^d) \iff (\mathcal{U}_{\mathcal{BFZ}} \psi) \in \mathcal{H}_\tau \cap H_{loc}^s(\mathbb{R}^d, L^2(\mathbb{T}^d))$;
- (ii) $\langle \mathbf{x} \rangle^s \psi \in L^2(\mathbb{R}^d), \forall s \in \mathbb{N} \iff (\mathcal{U}_{\mathcal{BFZ}} \psi) \in \mathcal{H}_\tau \cap C^\infty(\mathbb{R}^d, L^2(\mathbb{T}^d))$;
- (iii) $e^{\beta\|\cdot\|} \psi \in L^2(\mathbb{R}^d) \iff (\mathcal{U}_{\mathcal{BFZ}} \psi) \in \mathcal{H}_\tau \cap C^\omega(S_\beta, L^2(\mathbb{T}^d))$;
- (iv) $\psi \in H^s(\mathbb{R}^d) \iff (\mathcal{U}_{\mathcal{BFZ}} \psi) \in L^2(\mathbb{B}, H^s(\mathbb{T}^d))$.

Remark 1.2.9. Note that the point (ii) of Proposition 1.2.8 can be extended to fractional s by means of fractional Sobolev space theory, see [79] for more details on the subject.

In view of (1.2.8) we have that the set of Wannier functions $\{T_\gamma \psi_0\}_{\gamma \in \Gamma}$ is localized around the lattice centres in the sense that there exists a constant M , that does not depend on γ , such that

- (i) $\|\langle \cdot - \gamma \rangle^s \psi_\gamma\| \leq M \iff (\mathcal{U}_{\mathcal{BFZ}} \psi_0) \in \mathcal{H}_\tau \cap H_{loc}^s(\mathbb{R}^d, L^2(\mathbb{T}^d))$;
- (ii) $\|\langle \cdot - \gamma \rangle^s \psi_\gamma\| \leq M \forall s \in \mathbb{N} \iff (\mathcal{U}_{\mathcal{BFZ}} \psi_0) \in \mathcal{H}_\tau \cap C^\infty(\mathbb{R}^d, L^2(\mathbb{T}^d))$;
- (iii) $\|e^{\beta\|\cdot\|} \psi_\gamma\| \leq M \iff (\mathcal{U}_{\mathcal{BFZ}} \psi_0) \in \mathcal{H}_\tau \cap C^\omega(S_\beta, L^2(\mathbb{T}^d))$.

Nevertheless, there is one important consideration to do. The solution to the eigenvalue equation (1.2.6) is uniquely determined up to a phase factor. Indeed, the eigenvalue equation does not define a single eigenvalue problem but a family of eigenvalue problems. Therefore, the usual *phase-freedom* translates to what is called *Bloch gauge freedom*: for every $f : \mathbb{B} \rightarrow \mathbb{R}$, the function $e^{if(\mathbf{k})} \varphi_j(\mathbf{k})$, is again a Bloch function. As a consequence, the regularity of the Bloch functions and in turn the localization properties of the Wannier functions are determined by the choice of the gauge function f . For computational reasons, see [55], it is legitimate to ask for Wannier functions that are as localized as possible and this is equivalent to ask for Bloch functions that are as regular as possible. Nevertheless, this is not always possible and the obstruction to this fact has a precise topological meaning.

Notice that in the case that σ_0 is composed by m bands, and each band satisfies Assumption 1.2.4, one can simply iterate the construction made for the single band, see Remark 1.2.7.

As it is well discussed in the literature, see [2], the assumption of isolated Bloch bands is highly non physical. Indeed, in real solids the Bloch bands do intersect each other, thus it becomes necessary to develop a multi-band approach to overcome the problem.

In the previous paragraph we have seen that, in the case of isolated bands, the Bloch function is both eigenfunction of the fiber Hamiltonian $h(\mathbf{k})$ and of the fiber projection $P_0(\mathbf{k})$. Nevertheless, when band crossings are present and $d > 1$, we know from general perturbation theory [64] that already the eigenprojections onto the single band could not be smooth with respect to \mathbf{k} . Therefore, in order to find a well localized basis for the range of the fiber projection $P_0(\mathbf{k})$, one relaxes the notion of Bloch function.

Definition 1.2.10 (Bloch frames). Consider the families of \mathbf{k} dependent Hamiltonians $\{h(\mathbf{k})\}_{\mathbf{k} \in \mathbb{B}}$ and rank m projections $\{P_0(\mathbf{k})\}_{\mathbf{k} \in \mathbb{B}}$. Moreover, consider the family of \mathbf{k} orthonormal vectors $\{\varphi_i(\mathbf{k})\}_{\mathbf{k} \in \mathbb{B}, i=1, \dots, m}$. Then, we say that $\{\varphi_i(\mathbf{k})\}_{\mathbf{k} \in \mathbb{B}, i=1, \dots, m}$ is a *Bloch frame* for P_0 if for every \mathbf{k}

$$P_0(\mathbf{k})\varphi_i(\mathbf{k}) = \varphi_i(\mathbf{k}), \quad i = 1, \dots, m,$$

and the $\varphi_i \in \mathcal{H}_\tau$ are called *quasi-Bloch* functions. For any family of unitary $m \times m$ matrices $\{U(\mathbf{k})\}_{\mathbf{k} \in \mathbb{B}}$, the family of vectors $\{U(\mathbf{k})\varphi_i(\mathbf{k})\}_{\mathbf{k} \in \mathbb{B}, i=1, \dots, m}$ is still a Bloch frame for the family $\{P_0(\mathbf{k})\}_{\mathbf{k} \in \mathbb{B}}$.

Therefore, in view of the previous definition we define the composite Wannier functions.

Definition 1.2.11 (Composite Wannier function). We say that the set of vectors $\{T_\gamma \psi_{0,i}\}_{\gamma \in \Gamma, i=1, \dots, m}$ is an orthonormal basis of *composite Wannier functions* for the range of P_0 , if

$$\psi_{0,i} := \mathcal{U}_{\mathcal{BFZ}}^{-1} \varphi_i,$$

and $\{\varphi_i(\mathbf{k}), i = 1, \dots, m\}_{\mathbf{k} \in \mathbb{B}}$ is a *Bloch frame* for P_0 .

Remark 1.2.12. In some particular situations it might happen to have a Bloch frame in which the quasi-Bloch functions are also Bloch functions. Explicitly, the family of \mathbf{k} orthonormal vectors $\{\varphi_i(\mathbf{k})\}_{\mathbf{k} \in \mathbb{B}, i=1, \dots, m}$ is a Bloch frame of Bloch functions for P_0 if for every \mathbf{k}

$$h(\mathbf{k})\varphi_i(\mathbf{k}) = E_i(\mathbf{k})\varphi_i(\mathbf{k}), \quad P_0(\mathbf{k})\varphi_i(\mathbf{k}) = \varphi_i(\mathbf{k}), \quad i = 1, \dots, m.$$

Then, for any unitary matrix $U(\mathbf{k})$ of the form

$$(U(\mathbf{k}))_{ij} = \delta_{ij} e^{if_i(\mathbf{k})}, \quad i, j = 1, \dots, m,$$

where $f_i : \mathbb{B} \rightarrow \mathbb{R}$, $i = 1, \dots, m$ are generic real valued function, the set of vectors $\{U(\mathbf{k})\varphi_i(\mathbf{k})\}_{\mathbf{k} \in \mathbb{B}, i=1, \dots, m}$ is still a Bloch frame of Bloch functions for the family $\{P_0(\mathbf{k})\}_{\mathbf{k} \in \mathbb{B}}$. Accordingly, one has an orthonormal basis of Wannier functions for the range of P_0 , if

$$\psi_{0,i} := \mathcal{U}_{\mathcal{BFZ}}^{-1} \varphi_i,$$

and $\{\varphi_i(\mathbf{k}), i = 1, \dots, m\}_{\mathbf{k} \in \mathbb{B}}$ is a Bloch frame of Bloch functions for P_0 .

The objects described in Remark 1.2.12 are useful only when one deals with a group of separated single energy bands. Since this situation is very rare in the energy bands of topological insulators, in the following we will speak only about Bloch frames and composite Wannier functions, as defined in Definition 1.2.11 and Definition 1.2.10, sometimes omitting the adjective “composite”.

As a consequence of Proposition 1.2.8 the existence of a localized orthonormal basis made by composite Wannier functions is equivalent to the existence of a regular Bloch frame, where the correspondence between the adjective “localized” and “regular” is explained in Proposition 1.2.8.

1.2.2 Systems with constant magnetic field

The periodicity assumptions made in the previous paragraphs about the magnetic vector potential are such to exclude the case of a perfect crystal subjected to a constant magnetic field. This is a very inconvenient problem for a theory that aims to describe phenomena such as the Integer Quantum Hall Effect in which the presence of a constant magnetic field plays a crucial role. The problem can be solved by introducing the concept of magnetic translations [119], namely a set of unitary operators that depends on the value of the magnetic field, and that implements mathematically the *translational symmetry* of the system. Let us restrict for simplicity to dimension $d = 2$, $\Gamma = \mathbb{Z}^2$ and consider the Hamiltonian H_Γ defined in (1.2.1) to which we add a constant magnetic field of strength b and orthogonal to the plane \mathbb{R}^2 , that is

$$H_{\mathbb{Z}^2}^{(b)} = \frac{1}{2} (\mathbf{P} - \mathbf{A}_{\mathbb{Z}^2} - b\mathbf{A})^2 + V_{\mathbb{Z}^2}, \quad (1.2.9)$$

where \mathbf{A} is the magnetic vector in the symmetric gauge, that is

$$\mathbf{A}(\mathbf{x}) = \frac{1}{2}(-x_2, x_1).$$

We also assume that the spectrum of $H_{\mathbb{Z}^2}^{(b)}$ has a spectral island $\sigma_0(H_{\mathbb{Z}^2}^{(b)})$ and we denote by P_b the spectral projection onto $\sigma_0(H_{\mathbb{Z}^2}^{(b)})$. As it has been first recognized by Zak [119], the fibering of the Hamiltonian can be recovered if we assume that the magnetic field flux per unit area satisfies a certain rationality condition. Let us show this in details. In view of the underlying periodic structure of the problem, compare with the previous section, every point $\mathbf{x} \in \mathbb{R}^2$ can be uniquely decomposed as

$$\mathbf{x} = \gamma + \underline{x}, \quad \gamma \in \mathbb{Z}^2, \quad \underline{x} \in \Omega.$$

Moreover, let ϕ be the usual Peierls magnetic phase, namely

$$\phi(\mathbf{x}, \mathbf{y}) := \frac{1}{2}(x_2y_1 - x_1y_2).$$

Consider b^* such that, for every $b^* = 2\pi p/q$ for some p, q co-prime integer numbers and define the (*modified*) *magnetic translation* of vector $\eta \in \Gamma$, $\widehat{\tau}_{b^*, \eta}$, to be the following unitary operator

$$(\widehat{\tau}_{b^*, \eta}\psi)(\gamma + \underline{x}) := e^{-ib^*\eta_1\eta_2/2} e^{ib^*\phi(\gamma + \underline{x}, \eta)} \psi(\gamma - \eta + \underline{x}), \quad \forall \psi \in L^2(\mathbb{R}^2). \quad (1.2.10)$$

By direct computation one can see that the Hamiltonian commutes with the magnetic translations for every $\eta \in \mathbb{Z}^2$, namely $\widehat{\tau}_{b^*,\eta} H_{\mathbb{Z}^2}^{(b)} = H_{\mathbb{Z}^2}^{(b)} \widehat{\tau}_{b^*,\eta}$. Again by direct computation one can prove that the set $\{\widehat{\tau}_{b^*,\eta}\}_{\eta \in \mathbb{Z}^2}$ forms a unitary projective representation of the group \mathbb{Z}^2 , that is

$$\widehat{\tau}_{b^*,\eta} \widehat{\tau}_{b^*,\xi} = e^{-ib^* \eta_2 \xi_1} \widehat{\tau}_{b^*,\eta+\xi}, \quad \forall \eta, \xi \in \mathbb{Z}^2.$$

Restricting the set of magnetic translation to the enlarged lattice

$$\mathbb{Z}_{(q)}^2 := \left\{ \eta \in \mathbb{Z}^2 \mid \eta = (\gamma_1, q\gamma_2), \gamma \in \mathbb{Z}^2 \right\},$$

implies that $\{\widehat{\tau}_{b^*,\eta}\}_{\eta \in \mathbb{Z}_{(q)}^2}$ forms a true unitary representation of \mathbb{Z}^2 , that is

$$\widehat{\tau}_{b^*,\eta} \widehat{\tau}_{b^*,\rho} = \widehat{\tau}_{b^*,\eta+\rho}, \quad \forall \eta, \rho \in \mathbb{Z}_{(q)}^2.$$

Moreover let us denote by $\mathbb{Z}_{(q)}^{2*}$ the dual lattice of $\mathbb{Z}_{(q)}^2$ and by $\mathbb{B}_{(q)}$ and $\Omega_{(q)}$ the restricted and enlarged unit cells of $\mathbb{Z}_{(q)}^2$ and $\mathbb{Z}_{(q)}^{2*}$ respectively.

Whenever the Hamiltonian commutes with all the elements of a unitary representation of the group \mathbb{Z}^2 , we can follow the procedure delineated before and construct an unitary operator that is able to "diagonalize simultaneously" the Hamiltonian and the unitary representation of \mathbb{Z}^2 . However, it is important to recall that this procedure is not unique and in the literature one can find basically two different approaches with their respective transform, namely the Bloch–Floquet–Zak and the Bloch–Floquet transform. Both these transforms have their own peculiarities, see for example [77] for a review on the subject, and they are unitarily equivalent via an explicit unitary transformation, see Section 2.5.1 for more details. In this chapter we choose to write everything in terms of the Bloch–Floquet–Zak transform. However, in Chapter 2 we also show how to work with the Bloch–Floquet transform.

Let us now define the magnetic Bloch–Floquet–Zak transform. For every $\psi \in C_0^\infty(\mathbb{R}^2)$ we define the operator

$$(\mathcal{U}_{\mathcal{BFZ}}\psi)(\mathbf{k}, y) := \frac{1}{|\mathbb{B}_{(q)}|^{1/2}} \sum_{\eta \in \mathbb{Z}_{(q)}^2} e^{-i\mathbf{k} \cdot (y-\eta)} (\widehat{\tau}_{b^*,\eta}\psi)(y), \quad \mathbf{k} \in \mathbb{R}^2, y \in \mathbb{R}^2. \quad (1.2.11)$$

From (1.2.11) we see that

$$(\widehat{\tau}_{b^*,\eta}(\mathcal{U}_{\mathcal{BFZ}}\psi))(\mathbf{k}, y) = (\mathcal{U}_{\mathcal{BFZ}}\psi)(\mathbf{k}, y), \quad \forall \eta \in \mathbb{Z}_{(q)}^2, \quad (1.2.12)$$

$$(\mathcal{U}_{\mathcal{BFZ}}\psi)(\mathbf{k} + \eta^*, y) = e^{-i\eta^* \cdot y} (\mathcal{U}_{\mathcal{BFZ}}\psi)(\mathbf{k}, y), \quad \forall \eta^* \in \mathbb{Z}_{(q)}^{2*}, \quad (1.2.13)$$

where with a little abuse of notation in (1.2.12), the magnetic translation $\widehat{\tau}_{b^*,\eta}$ is intended to act only on the second variable. Then, let \mathfrak{h} be the Hilbert space of square integrable functions on Ω_q that satisfy the magnetic periodic boundary conditions (1.2.12) and let $\tau(\eta^*)$ be the unitary operator defined by $(\tau(\eta^*)g)(y) = e^{-i\eta^* \cdot y} g(y)$, for all $g \in \mathfrak{h}$. An easy computation shows that $\tau(\cdot) : \mathbb{Z}_{(q)}^{2*} \rightarrow \mathcal{B}(\mathfrak{h})$ is a unitary representation of the abelian group $\mathbb{Z}_{(q)}^{2*}$. Therefore we can introduce the Hilbert space

$$\mathcal{H}_\tau^{(b^*)} := \left\{ \psi \in L^2(\mathbb{R}^2, \mathfrak{h}) \mid f(\mathbf{k} + \eta^*) = \tau(\eta^*)\psi(\mathbf{k}), \forall \eta^* \in \mathbb{Z}_{(q)}^{2*} \right\} \simeq \int_{\mathbb{B}_{(q)}}^\oplus d\mathbf{k} \mathfrak{h}.$$

Then the magnetic Bloch–Floquet–Zak transform can be extended to the whole Hilbert space and one obtains a unitary operator between $L^2(\mathbb{R}^2)$ and $\mathcal{H}_\tau^{(b^*)}$ such that

$$\begin{aligned}\mathcal{U}_{\mathcal{BFZ}} : L^2(\mathbb{R}^2) &\longmapsto \int_{\mathbb{B}(q)}^\oplus d\mathbf{k} \mathfrak{h}, \\ \mathcal{U}_{\mathcal{BFZ}} H_{\mathbb{Z}^2}^{(b^*)} \mathcal{U}_{\mathcal{BFZ}}^* &= \int_{\mathbb{B}(q)}^\oplus d\mathbf{k} H_{\mathbb{Z}^2}^{(b^*),\tau}(\mathbf{k}), \\ \mathcal{U}_{\mathcal{BFZ}} P_{b^*} \mathcal{U}_{\mathcal{BFZ}}^* &= \int_{\mathbb{B}(q)}^\oplus d\mathbf{k} P_{b^*}^\tau(\mathbf{k}).\end{aligned}$$

Note that $H_{\mathbb{Z}^2}^{(b^*),\tau}(\mathbf{k})$ and $P_{b^*}^\tau(\mathbf{k})$ are smooth and τ -equivariant functions of \mathbf{k} , namely

$$P_{b^*}^\tau(\mathbf{k} + \eta^*) = \tau(\eta^*) P_{b^*}^\tau(\mathbf{k}) \tau(\eta^*)^*, \quad H_{\mathbb{Z}^2}^{(b^*),\tau}(\mathbf{k} + \eta^*) = \tau(\eta^*) H_{\mathbb{Z}^2}^{(b^*),\tau}(\mathbf{k}) \tau(\eta^*)^*,$$

for all $\eta^* \in \mathbb{Z}_{(q)}^{2*}$. Therefore all the results described before can be adapted to this magnetic setting simply substituting the usual translations with the magnetic translations defined by (1.2.10).

Remark 1.2.13. We want to emphasize that in the presence of a constant magnetic field, a (composite) Wannier basis for the range of the projection P_0 is built using the magnetic translations instead of the usual translations.

Remark 1.2.14. The perturbation by a constant magnetic field has a very singular character, see [86] and Section 2.4.2, and has to be handled with care. In this section we have shown how to deal with a particular value of a magnetic field and, as one can see from the definition of the magnetic Bloch–Floquet–Zak transform, the value of b modifies both the definition of the unitary transform and its target space, making the comparison between systems with different magnetic fields complicated. In Chapter 5 we show how it is possible to define a transform that can treat systems with different values of constant magnetic field.

1.2.3 Existence results

As it has been first realized by Nenciu [84, 86] for the special cases of a single isolated Bloch band in generic dimension, and then rigorously proved by Panati for the general case in [89], the construction of a smooth and periodic Bloch frame for a given projection is not always possible and the obstruction has a clear topological meaning. Indeed, given a projection P onto a spectral island of the Hamiltonian $H_\Gamma^{(b)}$ (possibly with $b = 0$) it is possible to define a vector bundle, known as *Bloch bundle* [89].

Definition 1.2.15 (Bloch bundle). Let $\{P(\mathbf{k})\}_{\mathbf{k} \in \mathbb{R}^d}$ be a family of projections satisfying the points (i) (resp. (ii)) and (iii) of Proposition 1.2.6. On the set $\mathbb{R}^d \times \mathcal{H}_\tau$ define the equivalence relation \sim by

$$(\mathbf{k}, \varphi) \sim (\mathbf{k}', \varphi') \iff (\mathbf{k}, \varphi) = (\mathbf{k}' + \gamma^*, \tau(\gamma^*)\varphi') \text{ for some } \gamma^* \in \Gamma^*$$

and denote the equivalence classes of \sim by $[\mathbf{k}, \varphi]$. Define the total space E by

$$E := \left\{ [\mathbf{k}, \varphi] \in \mathbb{R}^d \times \mathcal{H}_\tau / \sim \mid \varphi \in \text{Ran } P(\mathbf{k}) \right\}.$$

Moreover define the projection $\pi : E \rightarrow \mathbb{B}$ given by $\pi([\mathbf{k}, \varphi]) = \mathbf{k}$, where $\mathbf{k} \in \mathbb{B}$ is such that $\mathbf{k} = \underline{\mathbf{k}} + \gamma^*$, with $\gamma^* \in \Gamma^*$. Then one can check that the triple (E, B, π) defines a smooth (resp. analytic) vector bundle $E \xrightarrow{\pi} B$, which is called *Bloch bundle*.

The existence of a Bloch frame for the projection P is therefore equivalent to the existence of a continuous, non vanishing and periodic global section for the Bloch bundle associated to $\{P(\mathbf{k})\}_{\mathbf{k} \in \mathbb{R}^d}$, which in turns is equivalent to the topological triviality of the vector bundle in the category of smooth Hermitian vector bundle over $\mathbb{B}_{(q)}$. One can prove, see [89], that for vector bundles over smooth manifold in low dimension ($d \leq 3$), like $\mathbb{B}_{(q)}$ for example, the topological obstruction to the existence of a continuous, non vanishing and periodic global section is given by the non vanishing of the first Chern numbers, where the Chern numbers associated to P are defined by³

$$c(P)_{ij} = \frac{1}{2\pi i} \int_{\mathbb{B}_{(q)} ij} dk_i dk_j \operatorname{Tr}_{\mathcal{H}} (P(\mathbf{k}) [\partial_i P(\mathbf{k}), \partial_j P(\mathbf{k})]) \in \mathbb{Z}, \quad 1 \leq i < j \leq d.$$

Indeed, the following Theorem by Panati [89] gives a complete answer to the question about the existence of exponentially localized (composite) Wannier basis for time-reversal symmetric systems.

Theorem 1.2.16 ([89]). *Let $d \leq 3$ and consider the smooth (resp. analytic) Bloch bundle associated to $\{P(\mathbf{k})\}_{\mathbf{k} \in \mathbb{R}^d}$. Assume moreover that the Bloch bundle is time-reversal symmetric, that is there exists an antiunitary operator Θ called time-reversal operator such that*

$$\Theta^2 = \mathbf{1}, \quad P(-\mathbf{k}) = \Theta P(\mathbf{k}) \Theta^{-1}.$$

Then the Chern numbers $c_{ij}(P)$ are equal to zero and the Bloch bundle admits a smooth (resp. analytic on S_α) and periodic global section.

Remark 1.2.17. Notice that the time-reversal operator Θ in Theorem 1.2.16 obeys $\Theta^2 = \mathbf{1}$. Time-reversal operators with such property are called *bosonic time-reversal operators*. A more accurate physical model of electrons in a crystal would require to consider also the spin degrees of freedom of the electrons. In that case one needs to consider *fermionic time-reversal operators*, namely time-reversal operator Θ such that $\Theta^2 = -\mathbf{1}$. The same result of Theorem 1.2.16 is valid also when $\Theta^2 = -\mathbf{1}$, see [77, Theorem 2] for more details.

In Chapter 5 we give an interpretation of the topological obstructions in terms of *unitary matching matrices* together with a direct proof of the fact that the Chern numbers are integers. Most important, we provide an explicit algorithm that allows to build the smooth Bloch frame. As a by-product we obtain an explicit construction of the exponentially localized Wannier basis in the topological trivial cases.

1.2.4 The localization dichotomy for periodic gapped quantum systems

In 1984 Thouless proved [111] that the Wannier functions spanning a single Landau level cannot decay faster than $|\mathbf{x}|^{-2}$. Thouless' proof is based on the non vanishing

³Notice that in dimension $d = 2$ there is only one Chern number. Hence we use the simpler notation $c_{12}(P) =: c(P)$.

Hall current for a single Landau level. This work laid the foundations of the idea that the localization of Wannier functions is related to the transport properties of the systems. In particular one is tempted to interpret the dissipationless transport in the topologically non trivial phases as a consequence of the de-localization properties of the Wannier functions. In 2016, a work by Monaco, Panati, Pisante and Teufel [79] put on a firm mathematical ground this idea. Indeed, they proved a theorem for $2 \leq d \leq 3$, which for $d = 2$ reduces to the following statement.

Theorem 1.2.18 ([79]). *Consider a periodic gapped Hamiltonian $H_\Gamma^{(b)}$ of the form (1.2.9). Assume that $H_\Gamma^{(b)}$ satisfies Assumption 1.2.4. Let $\{P_0(\mathbf{k})\}_{\mathbf{k} \in \mathbb{R}^2}$ be the family of spectral projections associated to the local spectral islands $\sigma_0(\mathbf{k})$, $\mathbf{k} \in \mathbb{R}^2$. Then one can construct an orthonormal basis $\{w_{a,\gamma}\}_{1 \leq a \leq m, \gamma \in \Gamma}$ of $\text{Ran } P_0$, where*

$$P_0 = \mathcal{U}_{\mathcal{BFZ}}^{-1} \int_{\mathbb{B}}^{\oplus} d\mathbf{k} P_0(\mathbf{k}) \mathcal{U}_{\mathcal{BFZ}},$$

consisting of composite Wannier functions such that each Wannier functions $w_{a,\gamma}$ satisfies

$$\sup_{1 \leq a \leq m, \gamma \in \Gamma} \int_{\mathbb{R}^2} d\mathbf{x} \langle \mathbf{x} - \gamma \rangle^{2s} |w_{a,\gamma}(\mathbf{x})|^2 \leq M_s < +\infty, \quad \text{for every } s < 1,$$

where M_s is a positive constant independent of γ . Moreover, the following statements are equivalent:

- (a) *there exists a basis of composite Wannier functions $\{w_{a,\gamma}\}_{1 \leq a \leq m, \gamma \in \Gamma}$ with finite second moment, that is*

$$\sup_{1 \leq a \leq m, \gamma \in \Gamma} \int_{\mathbb{R}^2} d\mathbf{x} \langle \mathbf{x} - \gamma \rangle^2 |w_{a,\gamma}(\mathbf{x})|^2 \leq M_1 < +\infty,$$

where M_1 is a positive constant.

- (b) *There exists a basis of composite Wannier functions $\{w_{a,\gamma}\}_{1 \leq a \leq m, \gamma \in \Gamma}$ that are exponentially localized, namely there exists $\alpha > 0$ such that for all $0 < \beta < \alpha$*

$$\sup_{1 \leq a \leq m, \gamma \in \Gamma} \int_{\mathbb{R}^2} d\mathbf{x} e^{2\beta \|\mathbf{x} - \gamma\|} |w_{a,\gamma}(\mathbf{x})|^2 \leq \widetilde{M}_\beta < +\infty,$$

where \widetilde{M}_β is a positive constant.

- (c) *The Bloch bundle constructed from the family of projections $\{P_0(\mathbf{k})\}_{\mathbf{k} \in \mathbb{R}^2}$ is topologically trivial, that is $c(P_0) = 0$.*

As one can see directly from Theorem 1.2.18, the localization of Wannier functions presents a dichotomic behaviour: if the system is topologically trivial then one can not only find a Bloch gauge that makes second moment of the Wannier function being finite, but it is possible to find a Bloch gauge that makes the corresponding Wannier functions to be exponentially localized. On the contrary, if the system is topologically non trivial, in the sense that its Chern number is different from zero, then there is no chance to find a basis of Wannier functions with finite second

moment. In these terms, the topology of the Bloch bundle manifests itself as a “phase transition” on the localization of the Wannier functions. It is for these reasons that this result has been dubbed *localization dichotomy* in [79, 78]

As we mentioned in the Introduction, the long term goal of this work is the generalization of Theorem 1.2.18 for generic gapped quantum systems, without periodicity, taking this as a lodestar, in the next section we proceed by giving a precise definition of Wannier functions in the absence of a periodicity lattice.

1.3 Non periodic case: generalized Wannier functions

As it emerges from the previous sections, the definition of Wannier functions mainly relies on the existence of \mathbf{k} -space structure and a related fibered Hamiltonian. However, distilling the true essence of the concept of Wannier basis, one can say that it is a special basis capable of describing important transport and topological features of a certain spectral subspace of the original Hamiltonian. In this respect it is possible to ask for a generalization of the concept of Wannier basis for non periodic systems.

Historically, the first result on the construction of Wannier functions for non periodic systems has been obtained by Kohn and Onffroy in 1973 [68]. They considered a centrosymmetric one-dimensional periodic system with a bounded impurity at the centre of symmetry. Relying on the pioneering idea of des Cloizeaux of *band projection operator* [42, 41], that is the position operator X restricted to the range of the projection P on the subspace of interest, namely PXP , they proved the existence of exponentially localized Wannier-type functions. Motivated by this work, in 1982 Kivelson [65], extended the result of Kohn and Onffroy to more general type of disordered systems. In the paper by Kivelson there is an interesting statement that, in some sense, summarizes the true essence of the Wannier functions. Quoting Kivelson’s words [65]:

This definition [the one by des Cloizeaux] of the Wannier functions is intuitively appealing; the Wannier function is the "best" approximation to an eigenstate of the position operator that can be made out of states in the band [of interest].

The first mathematically rigorous result on the existence of Wannier-type functions can be found in the paper by G. Nenciu and A. Nenciu [82] in 1993. They consider fairly general time-symmetric gapped Hamiltonian operator in generic dimension and prove the existence of exponentially localized Wannier-type basis “by continuity”. The definition of generalized Wannier basis that we adopt hereafter is based on the definition given there. We will extensively review the approach of “existence by continuity” in Section 1.4 and in Chapter 5. After that, the most remarkable result came with a work by the same authors [83] in 1998. They proved that, in one dimension, basically every reasonable gapped quantum system admits a generalized Wannier basis.

All these works put in evidence that the definition of Wannier functions can be given directly in position space and therefore it is a legitimate question to ask whether Wannier functions (or at least some weaker version of them) exist even in

absence of periodicity. Let us summarize this discussion with a quote by G. Nenciu and A. Nenciu [82]:

Summing up all the known results, one is tempted to conjecture that for time-reversal-invariant Hamiltonians generalized Wannier bases exist for all bounded isolated parts of their spectra, irrespective for the periodicity properties.

This conjecture is still an open problem and we hope that this work could contribute with a step forward toward the solution of the problem.

Moreover, the take-home message that we get from the research line that starts with Thouless [111] and arrives at the more recent work [79], is that the localization properties of the Wannier functions reflects the topological and transport properties of the model taken into account. Therefore, having access to a generalized Wannier basis for non periodic materials could be an useful and interesting tool in order to understand their physical properties.

In the following we will provide a mathematically rigorous framework to all these concepts.

First let us start by defining the localization functions.

Definition 1.3.1 (Localization function). We say that a continuous function $G : [0, +\infty) \rightarrow (0, +\infty)$ is a *localization function* if $\lim_{\|\mathbf{x}\| \rightarrow +\infty} G(\|\mathbf{x}\|) = +\infty$ and there exists a constant C_G such that

$$G(\|\mathbf{x} - \mathbf{y}\|) \leq C_G G(\|\mathbf{x} - \mathbf{z}\|) G(\|\mathbf{z} - \mathbf{y}\|), \quad \forall \mathbf{x}, \mathbf{y}, \mathbf{z} \in \mathbb{R}^2. \quad (1.3.1)$$

Then, in order to leave the safer periodic world, we require some -mild- assumptions on the Hamiltonian operator.

Assumption 1.3.2 (Potentials regularity). The following assumptions hold:

- (i) The scalar potential V is in $L^2_{loc}(\mathbb{R}^2)$ with uniform L^2 bound, that is

$$\sup_{\mathbf{x} \in \mathbb{R}^2} \int_{|\mathbf{x}-\mathbf{y}| \leq 1} |V(\mathbf{y})|^2 d\mathbf{y} < \infty. \quad (1.3.2)$$

- (ii) The magnetic vector potential $\mathbf{A} : \mathbb{R}^2 \rightarrow \mathbb{R}^2$ is in $L^2_{loc}(\mathbb{R}^2, \mathbb{R}^2) \cap L^4_{loc}(\mathbb{R}^2, \mathbb{R}^2)$ with distributional derivative $\nabla \cdot \mathbf{A} \in L^2_{loc}(\mathbb{R}^2)$.

Assumption 1.3.3 (Properties of the Hamiltonian operator). We consider a Hamiltonian operator of the form

$$H_A := -\Delta_A + V,$$

where $-\Delta_A = (-i\nabla - \mathbf{A})^2$ is called the magnetic Laplacian. We require that the magnetic vector potential \mathbf{A} and the scalar potential V satisfy the assumptions described in Assumption 1.3.2. Furthermore, assume that

- H1. H_A is selfadjoint on a suitable dense domain $\mathcal{D}_A \subset L^2(\mathbb{R}^2)$;

H2. H_A has a spectral gap g , namely there exist two non empty sets $\sigma_0, \sigma_1 \subset \mathbb{R}$ and $E_{\pm} \in \mathbb{R}$ such that

$$\sigma(H_A) = \sigma_0 \cup \sigma_1$$

and

$$\sup \sigma_0 < E_- < E_+ < \inf \sigma_1. \quad (1.3.3)$$

We call *gap* the interval $g := (E_-, E_+)$. Let $\mu \in g$. We call P_{μ} the spectral projection onto σ_0 .

Note that we sometimes refer to P_{μ} also with the name of *Fermi projection*, reminding the many body interpretation as the projection onto the space of “occupied” states of the system.

Remark 1.3.4. Under Assumption 1.3.2, V is infinitesimally bounded with respect to the Laplacian, [98, Theorem XIII.96], and also with respect to $-\Delta_A$, [7, Theorem 2.4].

Recall that the Japanese bracket of \mathbf{x} is defined by,

$$\langle \mathbf{x} \rangle := \left(1 + \|\mathbf{x}\|^2\right)^{\frac{1}{2}}.$$

Then, if $\mathbf{B} = (B_1, B_2)$ is a vector of two commuting self-adjoint operators, by functional calculus, we define

$$\langle \mathbf{B} \rangle := \left(1 + B_1^2 + B_2^2\right)^{\frac{1}{2}}$$

to be the Japanese bracket of B .

Proposition 1.3.5. *If the Hamiltonian operator H_A satisfies Assumption 1.3.3, then the following statements hold:*

- (i) H_A is essentially selfadjoint on $C_0^\infty(\mathbb{R}^2)$.
- (ii) H_A is bounded from below.
- (iii) The operator

$$H(\alpha) := e^{i\alpha\langle \cdot \rangle} H e^{-i\alpha\langle \cdot \rangle} \quad (1.3.4)$$

defined for $\alpha \in \mathbb{R}$, admits an analytic continuation as an analytic family in the sense of Kato to a strip

$$S_{\alpha_0} := \{x + iy \in \mathbb{C} \mid |y| < \alpha_0\}, \quad (1.3.5)$$

for any $\alpha_0 > 0$.

Proof. The statement (i) and (ii) are proved in [73, Theorem 3].

Now consider the statement (iii). This is another well-known property and a proof of it can be found in [10]. Let us recall here the idea of the proof. By simple computation we get

$$\begin{aligned} e^{i\alpha\langle \cdot \rangle} H_A e^{-i\alpha\langle \cdot \rangle} &= -\Delta_A + V + 2\alpha \nabla \langle \mathbf{x} \rangle \cdot (-i\nabla - \mathbf{A}) \\ &\quad + i\alpha \Delta \langle \cdot \rangle + \alpha^2 |\nabla \langle \mathbf{x} \rangle|^2 \\ &=: -\Delta_A + V + L(\alpha). \end{aligned}$$

Since by Assumption 1.3.2 the potential V is infinitesimally bounded with respect to $-\Delta_A$, see Remark 1.3.4, in order to guarantee the analytic continuation properties we need only to show that $L(\alpha)$ is infinitesimally bounded w.r. to $-\Delta_A$ for every $\alpha \in \mathbb{R}$. Then, let $z \in \rho(-\Delta_A)$ such that $z = i\mu$ with $\mu \in \mathbb{R}$, and consider the following operator

$$L(\alpha)(-\Delta_A - z)^{-1} = \left[2\alpha \nabla \langle \mathbf{x} \rangle \cdot (-i\nabla - \mathbf{A}) + i\alpha \Delta \langle \mathbf{x} \rangle + \alpha^2 |\nabla \langle \mathbf{x} \rangle|^2 \right] (-\Delta_A - z)^{-1}. \quad (1.3.6)$$

Since $\nabla \langle \mathbf{x} \rangle$ and $|\nabla \langle \mathbf{x} \rangle|^2$ are bounded operators, we only need to study $(-i\nabla - \mathbf{A})(-\Delta_A - z)^{-1}$. For every $\varphi \in \mathcal{D}(-\Delta_A)$ we have that

$$\begin{aligned} & \langle (-i\nabla - \mathbf{A})(-\Delta_A - z)^{-1}\varphi, (-i\nabla - \mathbf{A})(-\Delta_A - z)^{-1}\varphi \rangle \\ &= \langle (-\Delta_A - z)^{-1}\varphi, \left((-i\nabla - \mathbf{A})^2 - z \right) (-\Delta_A - z)^{-1}\varphi \rangle \\ &+ \langle (-\Delta_A - z)^{-1}\varphi, z(-\Delta_A - z)^{-1}\varphi \rangle. \end{aligned}$$

Hence it follows that

$$\left\| (-i\nabla - \mathbf{A})(-\Delta_A - z)^{-1}\varphi \right\| \leq \frac{2}{|\mu|^{\frac{1}{2}}}.$$

Which in turns implies that

$$\left\| L(\alpha)(-\Delta_A - i\mu)^{-1} \right\| \leq C|\mu|^{-\frac{1}{2}}.$$

From [1, Proposition 2.42] we get that $L(\alpha)$ is infinitesimally bounded with respect to $-\Delta_A$, then we can conclude the proof applying [98, Problem XII.11] and [98, Lemma p.16]. \square

Under Assumption 1.3.2, the projection P_μ admits a jointly continuous integral kernel that is exponentially localized,

$$|P_\mu(\mathbf{x}; \mathbf{y})| \leq C e^{-\beta \|\mathbf{x} - \mathbf{y}\|}, \quad (1.3.7)$$

for some $\beta > 0$ and $C > 0$. This is a standard result [104, 19] in the theory of Schrödinger operators and it is basically a consequence of the gap condition and of the regularity of the potentials, see Assumption 1.3.2. The main tool needed to prove the exponential localization of P_μ is the theory of Combes–Thomas estimates. For the reader's convenience, in Section A.1.1 we review the Combes–Thomas theory and prove (1.3.7).

Following the idea in [83] we define the generalized Wannier functions.

Definition 1.3.6. P_μ admits a *generalized Wannier basis* (GWB) if there exist:

- (i) a Delone set $\mathfrak{D} \subseteq \mathbb{R}^2$, i. e. a discrete set such that $\exists 0 < r < R < \infty$:
 - (a) $\forall \mathbf{x} \in \mathbb{R}^2$ there is at most one element of \mathfrak{D} in the ball of radius r centred at \mathbf{x} (in particular, the set has no accumulation points);
 - (b) $\forall \mathbf{x} \in \mathbb{R}^2$ there is at least one element of \mathfrak{D} in the ball of radius R centred at \mathbf{x} (the set is not sparse);

- (ii) a localization function G , a constant $M > 0$ independent of $\gamma \in \mathfrak{D}$ and an orthonormal basis of $\text{Ran } P_\mu$, $\{\psi_{\gamma,a}\}_{\gamma \in \mathfrak{D}, 1 \leq a \leq m(\gamma) < \infty}$ with $m(\gamma) \leq m^* \forall \gamma \in \mathfrak{D}$, satisfying

$$\int_{\mathbb{R}^2} |\psi_{\gamma,a}(\mathbf{x})|^2 G(\|\mathbf{x} - \gamma\|) d\mathbf{x} \leq M.$$

We call $\psi_{\gamma,a}$ a *generalized Wannier function* (GWF) with *centre* γ .

The existence of a GWB implies that the integral kernel of P_μ can be written as

$$P_\mu(\mathbf{x}; \mathbf{y}) = \sum_{\gamma,a} \psi_{\gamma,a}(\mathbf{x}) \psi_{\gamma,a}(\mathbf{y}), \quad \forall \mathbf{x}, \mathbf{y} \in \mathbb{R}^2.$$

Using the usual “bra-ket” physicists notation it is possible to write the projection as

$$P_\mu = \sum_{\gamma,a} |\psi_{\gamma,a}\rangle \langle \psi_{\gamma,a}|$$

where the series has to be intended as the strong limit of the finite sums of projections on the one-dimensional spaces spanned by each GWF.

Notice that from the L^2 localization estimate in Definition 1.3.6 (ii) we can extract a L^∞ estimate using equation (1.3.7). Indeed, consider

$$\begin{aligned} \sup_{\mathbf{x} \in \mathbb{R}^2} \left| G(\|\mathbf{x} - \gamma\|)^{1/2} \psi_{\gamma,a}(\mathbf{x}) \right| &\leq \int_{\mathbb{R}^2} d\mathbf{y} G(\|\mathbf{x} - \gamma\|)^{1/2} |P_\mu(\mathbf{x}; \mathbf{y})| |\psi_{\gamma,a}(\mathbf{y})| \\ &\leq \int_{\mathbb{R}^2} d\mathbf{y} G(\|\mathbf{x} - \mathbf{y}\|)^{1/2} |P_\mu(\mathbf{x}; \mathbf{y})| G(\|\gamma - \mathbf{y}\|)^{1/2} |\psi_{\gamma,a}(\mathbf{y})| \\ &\leq \left(\int_{\mathbb{R}^2} d\mathbf{y} G(\|\mathbf{x} - \mathbf{y}\|) |P_\mu(\mathbf{x}; \mathbf{y})|^2 \right)^{1/2} \left(\int_{\mathbb{R}^2} d\mathbf{y} G(\|\gamma - \mathbf{y}\|) |\psi_{\gamma,a}(\mathbf{y})|^2 \right)^{1/2} \end{aligned}$$

where in the last equation we have used the Cauchy-Schwarz inequality. Thus, for every localization function G , such that $G(\|\mathbf{x}\|) \leq e^{\beta\|\mathbf{x}\|}$ where β satisfies (1.3.7), we have that there exists a positive constant C such that

$$\left(\int_{\mathbb{R}^2} d\mathbf{y} G(\|\mathbf{x} - \mathbf{y}\|) |P_\mu(\mathbf{x}; \mathbf{y})|^2 \right)^{1/2} \left(\int_{\mathbb{R}^2} d\mathbf{y} G(\|\gamma - \mathbf{y}\|) |\psi_{\gamma,a}(\mathbf{y})|^2 \right)^{1/2} \leq C.$$

Therefore we obtain the L^∞ estimate on the GWF

$$|\psi_{\gamma,a}(\mathbf{x})| \leq C G(\|\mathbf{x} - \gamma\|)^{-1/2}, \quad \text{for a.e. } \mathbf{x} \in \mathbb{R}^2. \quad (1.3.8)$$

Note that, a posteriori, the estimate (1.3.8) is true for every \mathbf{x} since the range of P_μ is contained in the domain of the Hamiltonian H_A , which in turn contains only continuous functions, see Section A.1.1. Let us introduce the following terminology:

- If the localisation function G is an exponential, that is $G(\|\mathbf{x}\|) = e^{2\alpha\|\mathbf{x}\|}$ for some $\alpha > 0$, then we say that the GWB is *exponentially localized*.
- If the localisation function G is of polynomial type, that is $G(\|\mathbf{x}\|) = \langle \mathbf{x} \rangle^{2s}$ for some $s > 0$, then we say that the GWB is *s-localized*.

It is straightforward to see that, whenever the GWB is exponentially localized, then it is also s -localized for every $s > 0$.

Remark 1.3.7. Definition 1.3.6 of generalized Wannier basis differs from the one given in [83] because of the requirement of \mathfrak{D} being a Delone set and because of the uniform bound m^* on the degeneracy of the eigenvalues. As one can see from Theorem 1.3.8, in [83] the lattice \mathfrak{D} coincides with the discrete spectrum of a particular selfadjoint operator and it is not defined as an independent object. Nevertheless, in view of the physical meaning of the irregular lattice \mathfrak{D} and of the eigenvalue degeneracy, we believe that this requirement has to be taken into account. We postpone to future investigations the study of the weakest assumptions on the potential V guaranteeing that the one-dimensional generalized Wannier basis constructed from the operator $\tilde{X} := P_\mu X P_\mu$, using the approach in [83], satisfies Definition 1.3.6.

Proving the existence of generalized Wannier functions in the full generality is not an easy problem. Currently there are only two articles about this problem. The already cited paper [83] in the one-dimensional setting and the work by Cornean, A. Nenciu and G. Nenciu [83] that deals with almost one-dimensional systems. In the first paper it is proved the existence of an exponentially localized basis of functions for the Fermi projection for one-dimensional systems, while in the second paper the construction is extended to systems in \mathbb{R}^d , $d \leq 3$, without magnetic field and with a confining potential of the following type. In dimension $d \leq 3$ consider a scalar potential V that satisfies the Assumption 1.3.2 and such that, setting the notation $\mathbb{R}^d \ni \mathbf{x} = (x_1, \mathbf{x}_\perp)$, it holds

$$\lim_{R \rightarrow \infty} \sup_{x_1 \in \mathbb{R}; |\mathbf{x}_\perp| \geq R} \int_{|\mathbf{x}-\mathbf{y}| \leq 1} d\mathbf{y} |V(\mathbf{y})| = 0.$$

More relevantly, in the work [35], the authors implicitly prove that the lattice of localization satisfies the properties (a) of the Delone set definition. In the following we will recall what is known about the existence of one-dimensional generalized Wannier basis.

Theorem 1.3.8 (Existence of 1D generalized Wannier basis,[83, 35]). *Consider the Hilbert space $L^2(\mathbb{R})$ and the Hamiltonian operator*

$$H = -\Delta + V$$

satisfying Assumption 1.3.3. Let P_0 be the projection on the spectral island σ_0 . Then

- (i) *The operator $\tilde{X} := P_0 X P_0$ is selfadjoint on the domain $H^1(\mathbb{R}) \cap \text{Ran} P_0$.*
- (ii) *\tilde{X} has purely discrete spectrum.*
- (iii) *The set of eigenfunctions of \tilde{X} , $\{\psi_{\lambda,i}\}_{\lambda \in \sigma(\tilde{X}), 1 \leq i \leq m(\lambda)}$ is an orthonormal basis for the range of P_0 .*
- (iv) *Each eigenfunction is exponentially localized around the value of its eigenvalue, i. e. there exist two positive constants M_1, α such that*

$$\left\| e^{\alpha|\cdot-\lambda|} \psi_{\lambda,i} \right\| \leq M_1 \quad \text{for all } 1 \leq i \leq m(\lambda).$$

(v) The density of the spectrum is uniformly bounded from above. Denote by $\#(I)$ the number of isolated points in the set I . Then there exists a positive constant M_2 such that

$$\# \left((-L, L) \cap \sigma(\tilde{X}) \right) \leq M_2 L.$$

Note that the orthonormal set in Theorem 1.3.8, that is $\{\psi_{i,\lambda}\}_{\lambda \in \sigma(\tilde{X}), 1 \leq \lambda \leq m(\lambda)}$, is not a generalized Wannier basis in the sense of Definition 1.3.6 for two reasons:

- (i) The proof of Theorem 1.3.8 does not show the existence of an upper bound on the multiplicity of the eigenvalues, namely the existence of the constant m^* in Definition 1.3.6.
- (ii) As it is clear from the statement of Theorem 1.3.8, the role of the lattice is played by the spectrum of \tilde{X} . However, the theorem only shows that the set has no accumulation points, but there is no proof regarding the “not too sparse” property.

These two facts are still open questions and we plan to work on them in the future.

Remark 1.3.9. A key step in the proof of Theorem 1.3.8 is to prove that \tilde{X} is a compact operator. Unfortunately, the compactness property is peculiar only for one-dimensional systems. Indeed, already in dimension $d = 2$, it is not necessarily true. Consider for example the 2-dimensional system

$$H_{\mathbb{Z}^2} = -\Delta + V_{\mathbb{Z}^2}$$

with $V_{\mathbb{Z}^2}$ smooth. Consider the family of translations in the direction $\mathbf{e}_2 := (0, 1)$, that is $\{T_{n\mathbf{e}_2}\}_{n \in \mathbb{N}}$. Therefore we have that $[\tilde{X}, T_{n\mathbf{e}_2}] = 0$ for every $n \in \mathbb{N}$. By functional calculus this implies that for every $\mu \in \mathbb{R}$

$$\left[(\tilde{X} - \mu)^{-1}, T_{n\mathbf{e}_2} \right] = 0. \quad (1.3.9)$$

The relation (1.3.9) is sufficient to prove that \tilde{X} cannot have a compact resolvent. Let us prove it by contradiction. Suppose that $(\tilde{X} - \mu)^{-1}$ is a compact operator and consider the sequence $\{\varphi_n\}_{n \in \mathbb{N}}$ defined by

$$\varphi_n = T_{n\mathbf{e}_2} \varphi$$

with $\varphi \in C_0^\infty(\mathbb{R}^2)$ and $\|\varphi\| \neq 0$. The sequence $\{\varphi_n\}_{n \in \mathbb{N}}$ is clearly bounded since $\|\varphi_n\| = \|\varphi\|$. Therefore, by definition of compact operator we can extract a subsequence from $\{(\tilde{X} - \mu)^{-1} \varphi_n\}_{n \in \mathbb{N}}$, that is $\{(\tilde{X} - \mu)^{-1} \varphi_{n_k}\}_{n_k \in \mathbb{N}}$ such that it is convergent in norm, namely $\lim_{k \rightarrow +\infty} (\tilde{X} - \mu)^{-1} \varphi_{n_k} = \psi$. Equation (1.3.9) implies that

$$\left\| (\tilde{X} - \mu)^{-1} \varphi_{n_k} \right\| = \left\| T_{n\mathbf{e}_2} (\tilde{X} - \mu)^{-1} \varphi \right\| = \left\| (\tilde{X} - \mu)^{-1} \varphi \right\|,$$

which does not depend on n . Hence it follows

$$\begin{aligned} \|\psi\|^2 &= \left\| (\tilde{X} - \mu)^{-1} \varphi \right\|^2 \\ &= \lim_{k \rightarrow +\infty} \langle \psi, (\tilde{X} - \mu)^{-1} \varphi_{n_k} \rangle = \lim_{k \rightarrow +\infty} \langle (\tilde{X} - \mu)^{-1} \psi, T_{n_k \mathbf{e}_2} \varphi \rangle = 0, \end{aligned}$$

which is absurd and thus $(\tilde{X} - \mu)^{-1}$ can not be a compact operator. This simple, but at the same time instructive example, shows that the strategy used in [83] cannot be generally extended to higher dimensions but a new approach is needed.

1.3.1 Importance of intertwining with translations

Every well posed generalization of a concept must include the starting point idea as a particular subcase. In this respect, we now show that the construction of a GWB presented in [83] reduces to the construction of a composite Wannier basis in the sense described above.

Consider a one-dimensional system that is periodic with respect to some regular lattice $\Gamma \subset \mathbb{R}$, so that the corresponding Hamiltonian operator is

$$H_\Gamma = -\Delta + V_\Gamma,$$

with H_Γ satisfying Assumption 1.3.3. Then, the Hamiltonian, together with its functions defined via functional calculus, commute with the set of translations $\{T_\gamma\}_{\gamma \in \Gamma}$. This implies that

$$T_\gamma \tilde{X} = \tilde{X} T_\gamma - \gamma P_\mu.$$

Thus, for every eigenvector ψ of \tilde{X} , namely $\tilde{X}\psi = \lambda\psi$, we have that

$$\tilde{X} T_\gamma \psi = (\lambda + \gamma) T_\gamma \psi.$$

This has two important implications. First, it implies that the spectrum $\sigma(\tilde{X})$ is Γ periodic, that is, if $\lambda \in \sigma(\tilde{X})$ then $\lambda + \gamma \in \sigma(\tilde{X})$ for all $\gamma \in \Gamma$. In particular, assume for simplicity that the generator of the lattice Γ has norm greater than one⁴, then Theorem 1.3.8 (iv) implies that the density of the number of points in the spectrum is bounded. Hence, defining the unit cell (that is actually an interval) by Ω , we have that

$$\# \left((-L, L) \cap \sigma(\tilde{X}) \right) = L \# \left(\Omega \cap \sigma(\tilde{X}) \right) < \infty.$$

Second, it implies that the orthonormal basis of generalized Wannier basis has a ladder structure, namely the eigenpairs are given by

$$\{\lambda + \gamma, T_\gamma \psi_{i,\lambda}\}_{\lambda \in \sigma(\tilde{X}) \cap \Omega, 1 \leq \lambda \leq m(\lambda), \gamma \in \Gamma}.$$

The Wannier functions are then exponentially localized around the points λ and we interpret this fact as the presence of the atoms in the crystal. Nevertheless, note that the symmetry of the Hamiltonian is given by the lattice Γ and not by the discrete set $\sigma(\tilde{X})$. This is coherent with the existence of composite lattices: usually there is more than one atom per unit cell and the positions of the atoms do not coincide with the points of the symmetry lattice.

In order to show that the generalized Wannier basis is actually a composite Wannier basis one still has to show that the generalized Wannier basis is “compatible” with the periodic structure. This result can be found in the master thesis of Costa [39].

⁴It is not a strict assumption, since if H_Γ is periodic with respect to Γ , it is periodic also with respect to the lattice $n\Gamma$, $n \in \mathbb{N}$.

Proposition 1.3.10 ([39]). *Assume that P_0 admits a generalized Wannier basis with eigenpairs of the form*

$$\{\lambda + \gamma, T_\gamma \psi_{i,\lambda}\}_{\{\lambda \in \sigma(\tilde{X}) \cap \Omega, 1 \leq i \leq m(\lambda)\}}, \quad \gamma \in \Gamma.$$

Then $\{\mathcal{U}_{\mathcal{BFZ}} \psi_{i,\lambda}\}_{\lambda \in \sigma(\tilde{X}) \cap \Omega, 1 \leq i \leq m(\lambda)}$ is a Bloch frame for the family $\{P_0(k)\}_{k \in \mathbb{B}}$ where

$$P_0 = \int_{\mathbb{B}}^{\oplus} dk P_0(k).$$

Even though a straightforward generalization of the work contained in [83] is not possible, see Remark 1.3.9, it is possible to exploit the same strategy in order to construct some kind of special basis for the range of the projection. A particular basis made of Wannier-like function has been defined by Prodan [96] in 2015 for time-reversal symmetric disordered systems in any dimension. In Chapter 3 we extend Prodan's construction in order to take into account also systems with magnetic fields and we provide an explicit construction of that special orthonormal basis for the lowest Landau level. Nevertheless, as we will extensively argue later, the existence of such a basis for the first Landau level shows that these functions are not capable to grasp the transport properties of the systems, in contrast with the (composite) Wannier functions [111, 79].

1.4 Impurities and almost periodic cases

The considerations made in the previous sections show that proving the existence of a generalized Wannier basis in the full generality is far from being an easy task. However, if one knows that the Fermi projection of a reference system admits a generalized Wannier basis, it is possible to prove the existence of a generalized Wannier basis for systems that are small perturbations of the reference one. This procedure is called *proof by continuity* and it is based on the existence of a Kato–Sz.-Nagy unitary that intertwines the Fermi projections of the two systems. The first proof of existence of a generalized Wannier basis by continuity goes back to the work of G. Nenciu and A. Nenciu [82] where they consider Hamiltonians without magnetic field, then the same type of proof has been extended in the case of perturbation of time-reversal symmetric Hamiltonian operators by a small magnetic field by Cornean, Herbst and G. Nenciu [30]. In Chapter 5 we will show how to extend the results of [30] starting from magnetic Schrödinger Hamiltonians. In this section we recall the proof of [82] explicitly considering unbounded perturbing potentials. The physical model we have in mind is the periodic crystal with a countable number of impurities that breaks the periodicity of the system. In general the impurities can be locally described by Coulomb-type potentials.

Theorem 1.4.1 ([82]). *Consider a family of Hamiltonians $\{H_\lambda\}_{\lambda \in [0,1]}$ where each H_λ is defined by*

$$H_\lambda := -\Delta + V + \lambda W,$$

and V, W satisfy Assumption 1.3.2. Assume that each Hamiltonian satisfies Assumption 1.3.3 and assume that there exists a constant ℓ such that the size of the spectral gap of the Hamiltonian H_λ , namely g_λ , is bounded from below, that is

$\inf_{\lambda \in [0,1]} g_s = \ell > 0$. If H_0 admits an exponentially localized GWB basis, then, for λ sufficiently small, also H_λ does.

Proof. The strategy of the proof is to show that, for λ sufficiently small, we can “unitarily transport” the generalized Wannier functions from the range of P_0 to the range of P_λ without losing their localization properties.

Let us show this in detail. Consider the spectrum of H_0 , that is σ_0 . Since H_0 is bounded from below, see Proposition 1.3.5, the spectral island $\sigma_0(H_0)$ is contained in a finite interval of length D . Then, consider a closed contour \mathcal{C} that encloses $\sigma_0(H_0)$, since the potential W is infinitesimally relatively bounded with respect to H_0 , we can apply [64, Theorem IV.3.16] together with [64, Theorem IV.2.14] and prove that there exists λ^* such that for $\lambda < \lambda^*$, the spectral islands $\sigma_0(H_\lambda)$ are enclosed in the same contour \mathcal{C} . We can assume (enlarging the contour if necessary) that the contour \mathcal{C} is such that

$$\inf_{\lambda \in [0, \lambda^*]} \inf_{E \in \sigma_0(H_\lambda), z \in \mathcal{C}} |E - z| \geq \frac{\ell}{4}.$$

Then, via the Riesz formula, the projections onto the spectral islands $\sigma_0(H_\lambda)$ can be written using the same positively oriented contour \mathcal{C} , that is

$$P_\lambda = \frac{i}{2\pi} \oint_{\mathcal{C}} dz (H_\lambda - z)^{-1}.$$

From the Combes–Thomas estimates, see Proposition A.1.4 we get that there exist two positive constants K and α such that

$$\sup_{\mathbf{a} \in \mathbb{R}^d} \sup_{z \in \mathcal{C}} \left\| e^{\alpha \langle \cdot - \mathbf{a} \rangle} (H_\lambda - z)^{-1} e^{-\alpha \langle \cdot - \mathbf{a} \rangle} \right\| \leq K. \quad (1.4.1)$$

Notice that the constant α can be chosen such that $e^{\alpha \langle \mathbf{x} \rangle} \leq c G_0(\|\mathbf{x}\|)^{\frac{1}{2}}$, for some $c > 0$. Moreover, from the fact that W is infinitesimally relatively bounded we have that

$$\sup_{z \in \mathcal{C}} \left\| W (H_0 - z)^{-1} \right\| \leq K'. \quad (1.4.2)$$

Then, using (1.4.2) we obtain the norm continuity of the projection with respect to the parameter λ

$$\|P_\lambda - P_0\| = \left\| \frac{\lambda}{2\pi} \oint_{\mathcal{C}} dz (H_\lambda - z)^{-1} W (H_0 - z)^{-1} \right\| \leq \lambda C.$$

Moreover we have

$$\begin{aligned} e^{\alpha \langle \cdot - \mathbf{a} \rangle} (P_\lambda - P_0) e^{-\alpha \langle \cdot - \mathbf{a} \rangle} &= \frac{\lambda}{2\pi} \oint_{\mathcal{C}} dz e^{\alpha \langle \cdot - \mathbf{a} \rangle} (H_\lambda - z)^{-1} e^{-\alpha \langle \cdot - \mathbf{a} \rangle} \\ &\quad \cdot W e^{\alpha \langle \cdot - \mathbf{a} \rangle} (H_0 - z)^{-1} e^{-\alpha \langle \cdot - \mathbf{a} \rangle}. \end{aligned}$$

Performing the Combes–Thomas rotation we get that $e^{\alpha \langle \cdot - \mathbf{a} \rangle} (H_\lambda - z)^{-1} e^{-\alpha \langle \cdot - \mathbf{a} \rangle} = (H_\lambda - z)^{-1} B$ where B is a bounded operator. Using both (1.4.1) and (1.4.2) we obtain

$$\sup_{\mathbf{a} \in \mathbb{R}^d} \left\| e^{\alpha \langle \cdot - \mathbf{a} \rangle} (P_\lambda - P_0) e^{-\alpha \langle \cdot - \mathbf{a} \rangle} \right\| \leq \lambda C. \quad (1.4.3)$$

Therefore, at the price of choosing a new λ^* smaller than the previous one, we have that $\|P_\lambda - P_0\| \leq \frac{1}{2}$ and we can therefore define the Kato–Sz.-Nagy operator via the formula

$$U_\lambda := \left(1 - (P_\lambda - P_0)^2\right)^{-1/2} \{P_\lambda P_0 + (1 - P_\lambda)(1 - P_0)\},$$

where the first square root factor has to be intended by means of the functional calculus for bounded operators. The operator U_λ is unitary and intertwines the two projections, namely

$$P_\lambda = U_\lambda P_0 U_\lambda^*.$$

Since, for every integer n , it holds

$$e^{\alpha\langle \cdot - \mathbf{a} \rangle} (P_\lambda - P_0)^n e^{-\alpha\langle \cdot - \mathbf{a} \rangle} = \left(e^{\alpha\langle \cdot - \mathbf{a} \rangle} (P_\lambda - P_0) e^{-\alpha\langle \cdot - \mathbf{a} \rangle}\right)^n,$$

from (1.4.3) we deduce that, for λ small enough,

$$\left\|e^{\alpha\langle \cdot - \mathbf{a} \rangle} U_\lambda e^{-\alpha\langle \cdot - \mathbf{a} \rangle}\right\| \leq C \quad (1.4.4)$$

where C is a positive constant that is independent of \mathbf{a} . We are now ready to prove the existence of the generalized Wannier basis for the range of P_λ . Consider the generalized Wannier basis of P_0 , namely $\{\psi_{\eta,b}\}_{\eta \in \mathfrak{D}_0, 1 \leq b \leq m(\eta) < +\infty}$ with localization function $G_0(\|\mathbf{x}\|) := e^{2\alpha_0\|\mathbf{x}\|}$, then

$$\{U_\lambda \psi_{\eta,b}\}_{\eta \in \mathfrak{D}_0, 1 \leq b \leq m(\eta) < +\infty} \quad (1.4.5)$$

is clearly an orthonormal basis for the range of P_λ . Moreover, for any exponential localization function $G_\lambda(\|\mathbf{x}\|)^{\frac{1}{2}} \leq e^{\alpha\langle \mathbf{x} \rangle}$ we have

$$\begin{aligned} & G_\lambda(\|\cdot - \eta\|)^{\frac{1}{2}} U_\lambda \psi_{\eta,b} \\ &= G_\lambda(\|\cdot - \eta\|)^{\frac{1}{2}} e^{-\alpha\langle \cdot - \eta \rangle} e^{\alpha\langle \cdot - \eta \rangle} U_\lambda e^{-\alpha\langle \cdot - \eta \rangle} e^{\alpha\langle \cdot - \eta \rangle} G_0(\|\cdot - \eta\|)^{-\frac{1}{2}} G_0(\|\cdot - \eta\|)^{\frac{1}{2}} \psi_{\eta,b}. \end{aligned}$$

Therefore, using (1.4.4), we obtain $\left\|G_\lambda(\|\cdot - \eta\|)^{\frac{1}{2}} U_\lambda \psi_{\eta,b}\right\| \leq C'$. Note that the positive constant C' does not depend on η . This prove that the set defined in (1.4.5) is actually a generalized Wannier basis. \square

As mentioned in the proof, the key idea is to show that it is possible to unitarily transport the Wannier functions from one systems to the other. The unitary responsible for the transport has to keep track of the centre of localization of the Wannier functions and therefore it has to be localized in space in the sense of (1.4.3). In the following chapters we will see that a finer notion of localization for the unitary will be of crucial importance for our results. Moreover, notice that the localization function of the perturbed system is bounded by the localization function of the unperturbed one, hence this suggests that the localization of the Wannier functions is stable under a suitable small perturbation. We will discuss this point in Chapter 4, in particular see Remark 4.2.3.

Remark 1.4.2. The main application of Theorem 1.4.1 is the case of a time-reversal symmetric H_0 commuting with a representation of the group \mathbb{Z}^d , that is when H_0 describes a periodic and time-reversal symmetric system. Then, as we have seen in the previous sections, H_0 always admits an exponentially localized Wannier basis and then Theorem 1.4.1 says that, in presence of mild disorder that does not close the gap, one can still construct a basis of exponentially localized generalized Wannier functions for the perturbed system.

The results presented so far show that the quest for the existence of generalized Wannier basis is reasonable since there are plenty of examples for which a generalized Wannier basis without any \mathbf{k} -space counterpart does exist.

Chapter 2

Chern number in position space

In this chapter we investigate the properties of the Chern number in position space from different perspectives. First, starting from the definition of Chern number in the periodic setting we define the Chern character. Then, we present a proof of the Středa formula: since the original argument presented in the work by Cornean, Nenciu and Pedersen [38] did not explicit all the technical details, we show them here for the sake of completeness. In the last section we provide a proof of the gap labelling theorem for Bloch–Landau Hamiltonians. The last part of the chapter is the fruit of a joint work with H. Cornean and D. Monaco [32].

2.1 From \mathbf{k} -space to position space

In the previous chapter, see Section 1.2.3, we have shown that the existence of a Wannier basis is tightly related to the geometric concept of Chern number. The Chern number is usually expressed in the \mathbf{k} -space, however, in order to generalize the localization dichotomy to non periodic systems, we are interested in understanding the Chern number without any reference to the underlying \mathbf{k} -space. The natural idea is to use the magnetic Bloch–Floquet–Zak transform in order to identify the counterpart of the Chern number in position space.

Let us start with a technical proposition that extend to the setting of Section 1.2.2 a result already proved in [91] for time-reversal symmetric Hamiltonians.

Proposition 2.1.1. *Consider a bounded selfadjoint operator A on $L^2(\mathbb{R}^2)$ such that it is fibered in the magnetic Bloch–Floquet–Zak representation and $A(\mathbf{k})$ is a trace class operator with $\mathrm{Tr}_{\mathfrak{h}} |A(\mathbf{k})| \leq C$ for every $\mathbf{k} \in \mathbb{B}_{(q)}$. Then the trace per unit cell of A exists and is given by*

$$\mathrm{Tr}(A\chi_{\Omega_{(q)}+\gamma}) = \frac{1}{|\mathbb{B}_{(q)}|} \int_{\mathbb{B}_{(q)}} d\mathbf{k} \mathrm{Tr}_{\mathfrak{h}} A(\mathbf{k}). \quad (2.1.1)$$

Correspondingly, the trace per unit volume of A , called $\mathcal{T}(A)$, exists and is given by

$$\lim_{L \rightarrow \infty} \frac{1}{|\Lambda_L|} \mathrm{Tr}(A\chi_L) = \frac{1}{4\pi^2} \int_{\mathbb{B}_{(q)}} d\mathbf{k} \mathrm{Tr}_{\mathfrak{h}} A(\mathbf{k}), \quad (2.1.2)$$

where Λ_L denotes the square of side length $2L$ centred in zero, that is $\Lambda_L := (-L, L]^2$.

Proof. Since A is a fibered operator, we have that $A = \widehat{\tau}_{b^*,\eta} A \widehat{\tau}_{b^*,-\eta}$ for every $\eta \in \mathbb{Z}_{(q)}^2$. Moreover, $\chi_{\Omega_{(q)}} = \widehat{\tau}_{b^*,\eta} \chi_{(\Omega_{(q)} + \eta)} \widehat{\tau}_{b^*,-\eta}$, hence

$$\mathrm{Tr}(A \chi_{\Omega_{(q)}}) = \mathrm{Tr}(A \widehat{\tau}_{b^*,\eta} \chi_{\Omega_{(q)}} \widehat{\tau}_{b^*,-\eta}) = \mathrm{Tr}(A \chi_{(\Omega_{(q)} + \eta)}). \quad (2.1.3)$$

Then, in order to evaluate the trace $\mathrm{Tr}_{\mathfrak{h}}(A \mathbf{1}_{\Omega_{(q)}})$ we need an orthonormal basis of $\mathrm{Ran} \chi_{\Omega_{(q)}} \subset L^2(\mathbb{R}^2)$. Consider the set of functions $\{g_{\gamma^*}\}_{\gamma^* \in \mathbb{Z}_{(q)}^{2*}}$, where

$$g_{\gamma^*}(\mathbf{x}) := \chi_{\Omega_{(q)}}(\mathbf{x}) e^{i\gamma^* \cdot \mathbf{x}}, \quad \gamma^* \in \mathbb{Z}_{(q)}^{2*}.$$

The set $\{g_{\gamma^*}\}_{\gamma^* \in \mathbb{Z}_{(q)}^{2*}}$ is clearly an orthonormal basis for $\mathrm{Ran} \chi_{\Omega_{(q)}}$. Moreover

$$(\mathcal{U}_{\mathcal{BFZ}} g_{\gamma^*})(\mathbf{k}, y) = \frac{1}{|\mathbb{B}_{(q)}|^{1/2}} e^{-i\mathbf{k} \cdot y} e^{i\gamma^* \cdot y} =: e_{\gamma^*}(\mathbf{k}, y),$$

hence for every fixed $\mathbf{k} \in \mathbb{B}_{(q)}$ the set of functions $\{e_{\gamma^*}(\mathbf{k}, \cdot)\}_{\gamma^* \in \mathbb{Z}_{(q)}^{2*}}$ is an orthonormal basis of \mathfrak{h} . Since $\mathcal{U}_{\mathcal{BFZ}}$ is a unitary transformation, it follows that

$$\begin{aligned} \mathrm{Tr}(A \chi_{\Omega_{(q)}}) &= \sum_{\gamma^* \in \mathbb{Z}_{(q)}^{2*}} \langle g_{\gamma^*}, A \chi_{\Omega_{(q)}} g_{\gamma^*} \rangle \\ &= \frac{1}{|\mathbb{B}_{(q)}|} \int_{\mathbb{B}_{(q)}} d\mathbf{k} \sum_{\gamma^* \in \mathbb{Z}_{(q)}^{2*}} \langle e_{\gamma^*}(\mathbf{k}, \cdot), A(\mathbf{k}) e_{\gamma^*}(\mathbf{k}, \cdot) \rangle_{\mathfrak{h}} \\ &= \frac{1}{|\mathbb{B}_{(q)}|} \int_{\mathbb{B}_{(q)}} d\mathbf{k} \mathrm{Tr}_{\mathfrak{h}} A(\mathbf{k}). \end{aligned} \quad (2.1.4)$$

For an arbitrary measurable subset $\Lambda \subset \Omega_q$, the same computation with $\chi_{\Omega_{(q)}}$ replaced by χ_{Λ} shows that

$$|\mathrm{Tr}(A \chi_{\Lambda})| \leq \frac{1}{|\mathbb{B}_{(q)}|} \int_{\mathbb{B}_{(q)}} d\mathbf{k} \mathrm{Tr}_{\mathfrak{h}} |A(\mathbf{k})| \leq C.$$

Therefore, since every Λ_L can be decomposed in the sum of a number of unit cells plus some remainders terms that are negligible with respect to the area of Λ_L , in the limit $L \rightarrow +\infty$ we have

$$\lim_{L \rightarrow \infty} \frac{1}{|\Lambda_L|} \mathrm{Tr}(A \chi_{\Lambda_L}) = \frac{1}{|\Omega_{(q)}| |\mathbb{B}_{(q)}|} \int_{\mathbb{B}_{(q)}} d\mathbf{k} \mathrm{Tr}_{\mathfrak{h}} A(\mathbf{k}).$$

□

Consider now the operator $\mathfrak{C} := i\Pi_0 [[X_1, \Pi_0], [X_2, \Pi_0]]$, where we denote by Π_0 the spectral projection onto an isolated spectral island of the magnetic Hamiltonian operator $H_{\mathbb{Z}^2}^{(b)}$ defined in (1.2.9). Under the general Assumption 1.3.3, \mathfrak{C} is a bounded selfadjoint operator because the commutators $[X_i, \Pi_0]$, $i \in \{1, 2\}$, are bounded operators due to the gap condition. Indeed, for every $\varphi \in C_0^\infty(\mathbb{R}^2)$, by means of the Riesz formula we obtain

$$[X_i, \Pi_0] \varphi = \frac{i}{2\pi} \oint_{\mathcal{C}} dz \left[X_i, \left(H_{\mathbb{Z}^2}^{(b)} - z \right)^{-1} \right] \varphi.$$

Notice that the Combes–Thomas estimate guarantees that $(H_{\mathbb{Z}^2}^{(b)} - z)^{-1} : \mathcal{D}(X_i) \rightarrow \mathcal{D}(X_i)$ is a bounded operator on the domain of X_i , which in turn assures that the commutator is well defined. Therefore we have

$$\begin{aligned} [X_i, \Pi_0] \varphi &= \frac{i}{2\pi} \int_{\mathcal{C}} dz (H_{\mathbb{Z}^2}^{(b)} - z)^{-1} [H_{\mathbb{Z}^2}^{(b)}, X_i] (H_{\mathbb{Z}^2}^{(b)} - z)^{-1} \varphi \\ &= \frac{1}{2\pi} \int_{\mathcal{C}} dz (H_{\mathbb{Z}^2}^{(b)} - z)^{-1} (-i\nabla - \mathbf{A}_{\mathbb{Z}^2} - b\mathbf{A})_i (H_{\mathbb{Z}^2}^{(b)} - z)^{-1} \varphi. \end{aligned}$$

Since $(-i\nabla - \mathbf{A}_{\mathbb{Z}^2} - b\mathbf{A})_i$ is infinitesimally bounded with respect to $H_{\mathbb{Z}^2}^{(b)}$ and the contour \mathcal{C} is a compact subset of $\rho(H_{\mathbb{Z}^2}^{(b)})$, there exists a positive constant C independent of φ such that $\|[X_i, \Pi_0] \varphi\| \leq C \|\varphi\|$. Hence the commutator $[X_i, \Pi_0]$ can be extended as a bounded operator to the whole Hilbert space. Then, in order to apply Proposition 2.1.1 we have to check that \mathfrak{C} is a fibered operator with uniformly trace-class fibers. This is an easy consequence of

$$[\widehat{\tau}_{b^*, \eta}, X_i] = -\eta_i \widehat{\tau}_{b^*, \eta},$$

which implies that

$$[\mathfrak{C}, \widehat{\tau}_{b^*, \eta}] = 0.$$

Considering that $\mathcal{U}_{\mathcal{BFZ}} \mathbf{X} \mathcal{U}_{\mathcal{BFZ}}^* = i\nabla_{\mathbf{k}}$ we obtain the explicit form of the operator $\mathfrak{C}(\mathbf{k})$, that is

$$\mathfrak{C}(\mathbf{k}) := -i\Pi_0^\tau(\mathbf{k}) [\partial_1 \Pi_0^\tau(\mathbf{k}), \partial_2 \Pi_0^\tau(\mathbf{k})].$$

The smoothness of $\Pi_0^\tau(\cdot)$ as a function of \mathbf{k} , see Proposition 1.2.6, assures that the operator in (2.1) is continuous in \mathbf{k} . Moreover, since $\Pi_0^\tau(\mathbf{k})$ projects onto a subspace of dimension m for every $\mathbf{k} \in \mathbb{B}_{(q)}$, we have

$$\begin{aligned} \sup_{\mathbf{k} \in \mathbb{B}_{(q)}} \text{Tr}_{\mathfrak{h}} |\mathfrak{C}(\mathbf{k})| &= \sup_{\mathbf{k} \in \mathbb{B}_{(q)}} \text{Tr}_{\Pi_0^\tau(\mathbf{k})_{\mathfrak{h}}} |\mathfrak{C}(\mathbf{k})| \\ &\leq \sup_{\mathbf{k} \in \mathbb{B}_{(q)}} m \|\mathfrak{C}(\mathbf{k})\|_{\mathfrak{h}} = \sup_{\mathbf{k} \in \mathbb{B}_{(q)}} m \|\mathfrak{C}(\mathbf{k})\|_{\mathfrak{h}} \leq C, \end{aligned}$$

where in the last inequality we used the norm continuity in \mathbf{k} of $\mathfrak{C}(\mathbf{k})$. Therefore all the hypothesis of Proposition 2.1.1 are satisfied and we get that

$$\begin{aligned} \lim_{L \rightarrow \infty} \frac{1}{|\Lambda_L|} 2\pi i \text{Tr} (\chi_L \Pi_0 [[X_1, \Pi_0], [X_2, \Pi_0]] \chi_L) \\ = \frac{1}{2\pi i} \int_{\mathbb{B}_{(q)}} d\mathbf{k} \text{Tr}_{\mathfrak{h}} (\Pi_0^\tau(\mathbf{k}) [\partial_1 \Pi_0^\tau(\mathbf{k}), \partial_2 \Pi_0^\tau(\mathbf{k})]). \end{aligned} \quad (2.1.5)$$

Remark 2.1.2. When a trace class operator A has a jointly continuous integral kernel, the trace of A can be expressed as an integral, that is

$$\text{Tr}(A) = \int_{\mathbb{R}^2} d\mathbf{x} A(\mathbf{x}; \mathbf{x}), \quad (2.1.6)$$

see [99, Lemma p.65]. Note that, when the diagonal elements of the integral kernel are periodic, namely

$$A(\mathbf{x}; \mathbf{x}) = A(\underline{x} + \gamma; \underline{x} + \gamma) = A(\underline{x}; \underline{x}), \quad \mathbf{x} = \underline{x} + \gamma, \quad \mathbf{x} \in \mathbb{R}^2, \underline{x} \in \Omega, \gamma \in \mathbb{Z}^2,$$

then the trace per unit volume becomes an integral over the unit cell Ω . Indeed, we have that

$$\mathcal{T}(A) := \lim_{L \rightarrow \infty} \frac{1}{|\Lambda_L|} \text{Tr}(\chi_L A \chi_L) = \lim_{L \rightarrow \infty} \frac{1}{|\Lambda_L|} \int_{\Lambda_L} A(\mathbf{x}; \mathbf{x}).$$

Let $[x]$ denote the integer part of x and define $[L]' := [L + 1/2] - 1/2$; from now on we consider $L > 1/2$. Due to the periodicity hypothesis, the square $\Lambda_{[L]'}$ can be precisely covered by $(2[L]')^2$ translated copies of the unit cell Ω , that is

$$\Lambda_{[L]'} = \bigcup_{\gamma \in (\mathbb{Z}^2 \cap \Lambda_{[L]'})} (\Omega + \gamma).$$

When $L \neq [L]'$, Λ_L cannot be covered precisely by an integer number of unit cells, however it holds that $|\Lambda_L \setminus \Lambda_{[L]'}| \leq 4([L]' + 1)$. Therefore,

$$\begin{aligned} & \lim_{L \rightarrow \infty} \frac{1}{|\Lambda_L|} \int_{\Lambda_L} A(\mathbf{x}; \mathbf{x}) \\ &= \lim_{L \rightarrow \infty} \frac{1}{|\Lambda_{[L]'}| + |\Lambda_L \setminus \Lambda_{[L]'}|} \left(\int_{\Lambda_{[L]'}} A(\mathbf{x}; \mathbf{x}) + \int_{\Lambda_L \setminus \Lambda_{[L]'}} A(\mathbf{x}; \mathbf{x}) \right) \quad (2.1.7) \\ &= \int_{\Omega} d\mathbf{x} A(\mathbf{x}; \mathbf{x}) \end{aligned}$$

where in the last equality we have used that $\lim_{L \rightarrow \infty} \frac{|\Lambda_L \setminus \Lambda_{[L]'}|}{|\Lambda_{[L]'}|} = 0$ and the continuity of the integral kernel of A , so that $\left| \int_{\Lambda_L \setminus \Lambda_{[L]'}} A(\mathbf{x}; \mathbf{x}) \right| \leq C[L]'$.

Then, following a long path of scientific contributions (whose list will be detailed later), we find natural to set the following definition of *Chern character*.

Definition 2.1.3 (Chern character). Let P be a spectral projection, the *Chern character* of P is defined by

$$C(P) := \lim_{L \rightarrow \infty} \frac{2\pi}{4L^2} \text{Tr} (i\chi_L P [[X_1, P], [X_2, P]] P \chi_L), \quad (2.1.8)$$

whenever the limit on the right exists.

Definition 2.1.3 naturally suggests some questions.

1. Which are the conditions that guarantee that the Chern character is well defined and an integer quantity?
2. When the system is time-reversal symmetric but non-periodic, does the Chern number vanish?
3. The Chern character is a function of the Fermi projection. What happens when the Hamiltonian is perturbed? Does the Chern number change or is it a *stable* (in some precise sense that has to be defined) quantity?
4. The Chern number is related to the transport properties of the system, in particular is proportional to the Hall conductivity [112, 105]. Does the Chern character have some physical meaning in non periodic systems?

In this thesis we address all the questions above, in particular:

1. In Chapter 4 we prove that under very mild hypothesis on the Hamiltonian, namely Assumption 1.3.3, the existence of a well localized generalized Wannier basis implies that the Chern character is well defined and is zero. In Section 2.4 we show that a periodic Hamiltonian perturbed by a magnetic field (possibly with irrational value of the corresponding flux) has a well defined and integer valued Chern character.
2. In Section 2.3 we show that the Chern number vanishes whenever the Hamiltonian satisfies Assumption 1.3.3 and it is time-reversal symmetric.
3. In Section 2.4 we prove that the Chern character is stable under perturbation by a constant magnetic field. As a by-product of our proof we obtain that whenever two projections are Kato–Sz.-Nagy unitarily equivalent with a well localized unitary, they have the same Chern character.
4. In Section 2.2 we provide an alternative proof of the relation between transverse conductivity and Chern character, namely the well-known Středa formula. After that, in Section 2.4 we show that the Chern character can be interpreted as the response coefficient of the integrated density of states with respect to constant magnetic perturbations.

Remark 2.1.4. Some of these issues have been already addressed by different people and interesting results can be found in the literature in various contexts. In the next sections we will try to make a comparison with the existing literature, see Remark 2.2.2 and Section 2.4.1.

2.2 Středa formula and Chern character

Consider the setting of [38], that we briefly recall here for the reader's convenience.

We are interested in studying the behaviour of a 2-dimensional Fermi gas subjected to a constant magnetic field orthogonal to the plane. The one-electron dynamics in the Hilbert space $L^2(\mathbb{R}^2)$ is described by the Hamiltonian operator ¹

$$H_b := -\frac{1}{2}\Delta_A + V, \quad (2.2.1)$$

where

$$-\Delta_A = (-i\nabla - b\mathbf{A})^2 =: \mathbf{P}_A^2, \quad (2.2.2)$$

$b \in \mathbb{R}$ and \mathbf{A} is a magnetic vector potential in the symmetric gauge that is $\mathbf{A}(x_1, x_2) = \frac{1}{2}(-x_2, x_1)$. We set $b = -\frac{1}{c}\mathbf{B}$, where \mathbf{B} is the strength of the physical magnetic field and c is the speed of light. Moreover assume that the scalar potential V is \mathbb{Z}^2 -periodic, smooth and has uniformly bounded derivatives and the Hamiltonian H_b satisfies Assumption 1.3.3, in particular it has a spectral gap. We denote by $\Pi_0^{(b)}$ the projection onto the isolated spectral island $\sigma_0(H_b)$. Note that, as before, every point $\mathbf{x} \in \mathbb{R}^2$ can be uniquely decomposed as

$$\mathbf{x} = \gamma + \underline{x}, \quad \gamma \in \mathbb{Z}^2, \quad \underline{x} \in (-1/2, 1/2]^2 =: \Omega. \quad (2.2.3)$$

¹We use the Hartree units system $\hbar = 1 = e = m_e$.

In the following we often make use of this decomposition. Define the *magnetic translations*² as

$$(\tau_{b,\gamma}\psi)(\mathbf{x}) := e^{ib\phi(\mathbf{x},\gamma)}\psi(\mathbf{x} - \gamma), \quad \forall \psi \in L^2(\mathbb{R}^2), \quad (2.2.4)$$

where $\phi(\mathbf{x}, \mathbf{y}) := \frac{1}{2}(x_2y_1 - x_1y_2)$ is the usual Peierls magnetic phase. Since the potential V is periodic with respect to the lattice \mathbb{Z}^2 , that is $V(x + \gamma) = V(x)$ for every $\gamma \in \mathbb{Z}^2$, we have that the Hamiltonian commutes with the magnetic translations defined in (2.2.4). The Fermi projection has a jointly continuous integral kernel, see Section A.1, and, due to the commutation with the magnetic translations, it satisfies

$$\Pi_0^{(b)}(\mathbf{x}; \mathbf{x}') = e^{ib\phi(\mathbf{x},\gamma)}\Pi_0^{(b)}(\mathbf{x} - \gamma; \mathbf{x}' - \gamma)e^{-ib\phi(\mathbf{x},\gamma)}.$$

Therefore, in view of Remark 2.1.2, the integrated density of states $\mathcal{I}(\Pi_0^{(b)})$ of $\Pi_0^{(b)}$, defined by the trace per unit volume of the Fermi projection, is given by:

$$\mathcal{I}(\Pi_0^{(b)}) := \mathcal{T}(\Pi_0^{(b)}) = \int_{\Omega} d\mathbf{x} \Pi_0^{(b)}(\mathbf{x}; \mathbf{x}),$$

where we have highlighted the magnetic field dependence with the superscript “(b)”.

Let us now describe the Fermi gas. Consider a system of independent electrons in the grand canonical ensemble, namely assume that the physical system is in the thermodynamic equilibrium with a reservoir, which can exchange particles and energy with the system. More precisely, consider the family of square boxes $\{\Lambda_L\}_{L \geq 1}$ with the convention used before. The one particle Hilbert space is $L^2(\Lambda_L)$ and the one particle Hamiltonian is denoted by $H_b^{(L)}$ and is given by (2.2.1) restricted to Λ_L with Dirichlet boundary conditions, see [38] for a more precise discussion about this. Assume that the temperature $T = \frac{1}{k\beta}$, where k is the Boltzmann constant, and the chemical potential μ are fixed by a reservoir of energy and particles. Without entering into the details about the grand canonical ensemble and the Fock space formalism (mainly because we are not performing any thermodynamic limit and we defer the interested reader to [38] for more precise statements), assume that at time $t = -\infty$ the system is at equilibrium with the reservoir and the perturbation is adiabatically switched on until $t = 0$. The corresponding time-dependent Hamiltonian operator is

$$H_b^{(L)}(t) = H_b^{(L)} + V(t),$$

where the time dependent potential is given by

$$V(\mathbf{x}, t) = (e^{i\omega t} + e^{-i\omega t})E\mathbf{x}_2, \quad t \leq 0, \mathbf{x} \in \Lambda_L, \Im\omega < 0, E \in \mathbb{R}.$$

Notice that the role of the adiabatic parameter is played by the imaginary part of ω , namely $\Im\omega$. The state of the system is described by a time dependent density matrix $\rho(t)$ that satisfies the Liouville equation

$$i\partial_t \rho(t) = [H_b^{(L)}(t), \rho(t)], \quad \rho(-\infty) = f_{FD}(H_b^{(L)}),$$

²Note that the magnetic translations $\tau_{b,\gamma}$ defined in (2.2.4) and the modified magnetic translations $\widehat{\tau}_{b,\gamma}$ defined in (1.2.10), differ only by a phase factor.

where f_{FD} denotes the Fermi-Dirac distribution

$$f_{FD}(x) := \frac{1}{e^{\beta(x-\mu)} + 1}, \quad x \in \mathbb{R}, \beta > 0, \mu \in \mathbb{R}. \quad (2.2.5)$$

In the interaction picture and using the Dyson expansion one can argue that the solution to the Liouville equation is given by

$$\rho(0) = f_{FD}(H_b^{(L)}) - i \int_{-\infty}^0 [V^I(s), f_{FD}(H_b^{(L)})] ds + \mathcal{O}(E^2),$$

where $V^I(t) := e^{itH_b^{(L)}} V(t) e^{-itH_b^{(L)}}$. The current density that flows through the system at $t = 0$ is given by

$$\begin{aligned} \mathbf{j}^{(L)} &= \frac{i}{|\Lambda_L|} \text{Tr}_{L^2(\Lambda_L)} \left(f_{FD}(H_b^{(L)}) [\mathbf{X}, H_b^{(L)}] \right) \\ &+ \frac{1}{|\Lambda_L|} \text{Tr}_{L^2(\Lambda_L)} \left(\int_{-\infty}^0 [V^I(s), f_{FD}(H_b^{(L)})] ds [\mathbf{X}, H_b^{(L)}] \right) + \mathcal{O}(E^2). \end{aligned} \quad (2.2.6)$$

The conductivity tensor is therefore given by the first order coefficient of the current density expansion in E . Since we are interested in the transverse conductivity, we consider only the first component of the current density, namely \mathbf{j}_1 and we have (see [38] for more details)

$$\begin{aligned} \sigma^{(L)}(\mathbf{B}, T, \omega) &:= \sigma_{12}^{(L)} \\ &= -\frac{i}{|\Lambda_L|} \text{Tr}_{L^2(\Lambda_L)} \left(\int_{-\infty}^0 \left[e^{isH_b^{(L)}} X_2 e^{-isH_b^{(L)}}, (\mathbf{P}_A)_1 \right] f_{FD}(H_b^{(L)}) e^{is\omega} ds \right). \end{aligned}$$

In [38] and [37], it is proved that the conductivity admits a thermodynamic limit [38, Theorem 3.1] given by

$$\sigma(\mathbf{B}, T, \omega) := \lim_{L \rightarrow \infty} \sigma^{(L)}(\mathbf{B}, T, \omega) = -\frac{1}{2\pi\omega} \int_{\Omega} d\mathbf{x} \left[\int_{\Gamma_{\beta, \omega}} f_{FD}(z) \Sigma(z, \omega) dz \right] (\mathbf{x}; \mathbf{x}) \quad (2.2.7)$$

where

$$\begin{aligned} \Sigma(z, \omega) &:= (\mathbf{P}_A)_1 (H_b - z)^{-1} (\mathbf{P}_A)_2 (H_b - z - \omega)^{-1} \\ &+ (\mathbf{P}_A)_1 (H_b - z + \omega)^{-1} (\mathbf{P}_A)_2 (H_b - z)^{-1}, \end{aligned} \quad (2.2.8)$$

and $\Gamma_{\beta, \omega}$ is the anticlockwise oriented contour in the complex plane defined by

$$\Gamma_{\beta, \omega} := \{x \pm id \mid a \leq x \leq +\infty\} \cup \{a \pm iy \mid -d \leq y \leq d\}, \quad d := \min \left\{ \frac{\pi}{2\beta}, \frac{|\Im \omega|}{2} \right\},$$

where a is a lower bound on the spectrum of H_b , see Figure 2.1.

After that, the authors of [38] prove the so called Středa formula [110], namely that the limit $\omega \rightarrow 0$ of the transverse conductivity (that hereafter we call simply transverse conductivity), in the limit zero temperature, is given by the derivative of the integrated density of states with respect to the magnetic field:

$$\lim_{\omega \rightarrow 0} \lim_{T \rightarrow 0} \sigma(\mathbf{B}_0, T, \omega) = \left. \frac{d\mathcal{I}(\Pi_0^{(b)})}{db} \right|_{b=b_0}. \quad (2.2.9)$$

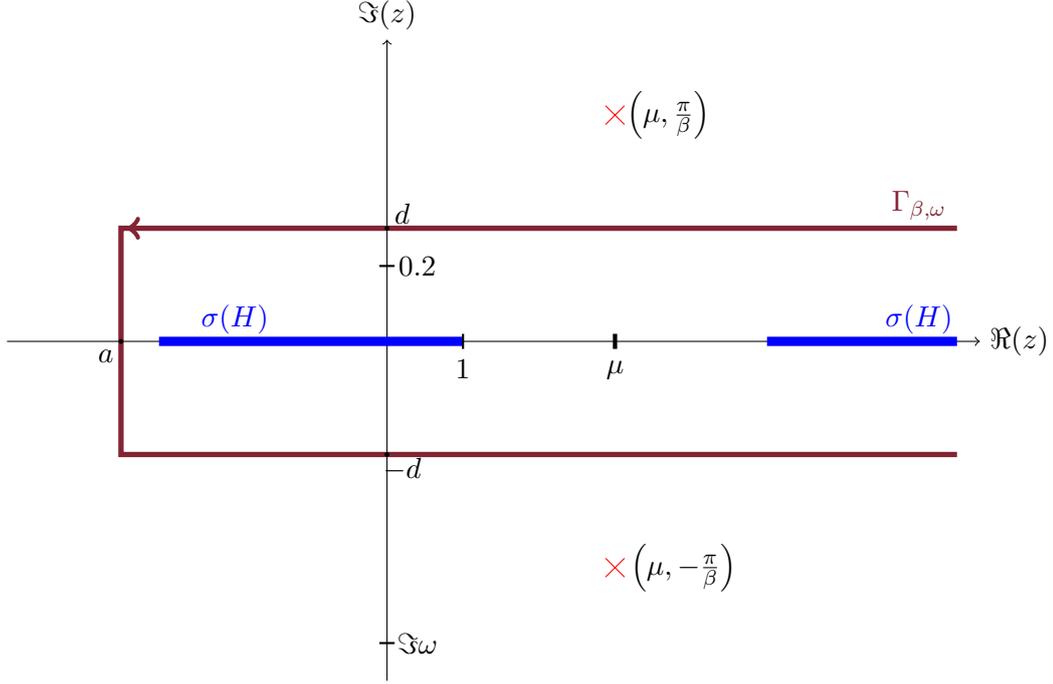


Figure 2.1. Graphical representation of the contour $\Gamma_{\beta,\omega}$. Note that the length scale used on the imaginary axis is $1/5$ of the length scale used on the real axis.

The derivation carried out in [38] for (2.2.7) is made for three dimensional systems, taking into account also the spin degrees of freedom. Moreover, in the proof of equation (2.2.9), contained in [38], there are some steps that are not completely detailed. Assuming that the result for the thermodynamic limit of the conductivity, that is (2.2.7), holds true also for two dimensional systems, we show here a detailed proof of the Středa formula adapting the techniques presented in [37] and we show that the transverse conductivity is proportional to the Chern character of the Fermi projection.

Theorem 2.2.1. *Assume that the formula for the thermodynamic limit of the transverse conductivity (2.2.7) holds true in dimension $d = 2$. Then, taking first the limit $T \rightarrow 0$ and then $\omega \rightarrow 0$, one gets*

$$\frac{C(\Pi_0^{(b_0)})}{2\pi} = \lim_{\omega \rightarrow 0} \lim_{T \rightarrow 0} \sigma(b_0, T, \omega) = \left. \frac{d\mathcal{I}(\Pi_0^{(b)})}{db} \right|_{b=b_0},$$

where $C(\Pi_0^{(b_0)})$ is the Chern character of the Fermi projection $\Pi_0^{(b_0)}$, see Definition 2.1.3.

Remark 2.2.2. In the context of our work, this result is of fundamental importance: it provides a rigorous mathematical connection between the position space Chern number and the transport properties of the systems when there is no \mathbf{k} -space involved. Note that the result is not new. Indeed, it first appeared in the context of discrete systems in the work by Bellissard, van Elst and Schulz-Baldes [15]

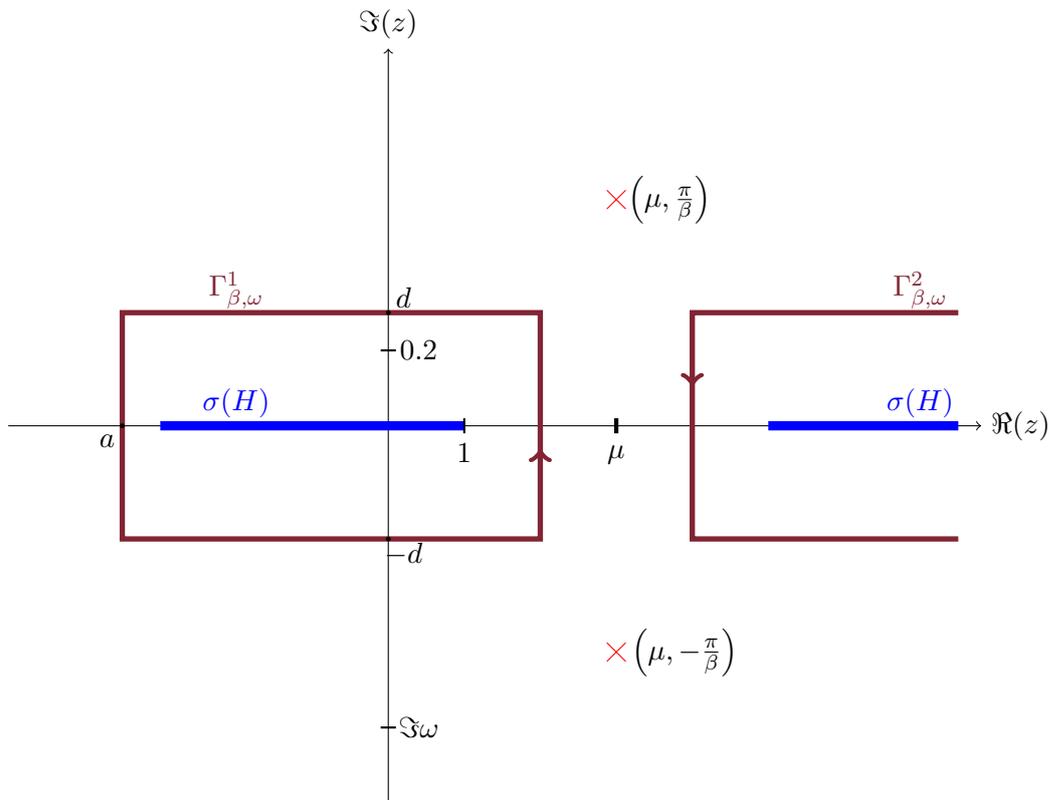


Figure 2.2. Graphical representation of the contours $\Gamma_{\beta,\omega}^1$ and $\Gamma_{\beta,\omega}^2$. Note that the length scale used on the imaginary axis is $1/5$ of the length scale used on the real axis.

and subsequently the first equality has been rigorously proved also in the case of unbounded operators, see the paper by Bouclet, Germinet, Klein and Schenker [18] and the more recent book by De Nittis and Lein [40]. In addition, recently there has been important rigorous results regarding the quantization of Hall conductance for interacting electrons systems, see the paper by Hastings and Michalakis [60], the work by Giuliani, Mastropietro and Porta [54], the paper by Giuliani, Jauslin, Mastropietro and Porta [53] and the work by Monaco and Teufel [81].

However, we want to emphasize that this is the first derivation of the Středa formula considering the limit of zero temperature and zero frequency. We consider this result in view of future further investigation about the role of topology and the behaviour of topological insulators at finite temperature.

2.2.1 Proof of Theorem 2.2.1

Consider the formula for the conductivity (2.2.7). Due to the gap in the spectrum, for $|\omega| < g := \frac{E_+ - E_-}{4}$, we can replace the integral over z on the contour $\Gamma_{\beta,\omega}$ with

the integral on the anticlockwise contour $\Gamma_{\beta,\omega}^1 \cup \Gamma_{\beta,\omega}^2$ where

$$\begin{aligned}\Gamma_{\beta,\omega}^1 &:= \{x \pm id \mid a \leq x \leq E_- + g\} \cup \{a + iy \mid -d \leq y \leq d\} \\ &\quad \cup \{E_- + g + iy \mid -d \leq y \leq d\}; \\ \Gamma_{\beta,\omega}^2 &:= \{x \pm id \mid x \geq E_- + g\} \cup \{E_+ - g + iy \mid -d \leq y \leq d\},\end{aligned}$$

see Figure 2.2.

In view of this decomposition of the contour $\Gamma_{\beta,\omega}$, we have

$$\begin{aligned}\sigma(b, T, \omega) = -\frac{1}{2\pi\omega} \int_{\Omega} d\mathbf{x} &\left[\int_{\Gamma_{\beta,\omega}^1} \Sigma(z, \omega) dz + \right. \\ &\left. \int_{\Gamma_{\beta,\omega}^1} (f_{FD}(z) - 1) \Sigma(z, \omega) dz + \int_{\Gamma_{\beta,\omega}^2} f_{FD}(z) \Sigma(z, \omega) dz \right] (\underline{x}; \underline{x}).\end{aligned}\tag{2.2.10}$$

Since the new contour, namely $\Gamma_{\beta,\omega}^1 \cup \Gamma_{\beta,\omega}^2$, does not intersect the singularity line (the singularities of the Fermi-Dirac distribution (2.2.5) all lie on the line³ $\mu + iy$, $y \in (-\infty, +\infty)$), we can choose $\Gamma_{\beta,\omega}^1 \cup \Gamma_{\beta,\omega}^2$ to be independent of β simply setting $d = \frac{|\Im(\omega)|}{2}$, we call these new contours Γ_{ω}^1 and Γ_{ω}^2 .

We are now ready to perform the limit $\beta \rightarrow \infty$, which corresponds to $T \rightarrow 0$. First of all notice that all the three operators in the square bracket in equation (2.2.10) have a jointly continuous integral kernel. Indeed, consider the two operators defined by the closed complex contour Γ_{ω}^1 . Integrating by parts with respect to the complex variable z one obtains

$$\begin{aligned}&\int_{\Gamma_{\omega}^1} \Sigma(z, \omega) dz \\ &= - \int_{\Gamma_{\omega}^1} dz z (\mathbf{P}_A)_1 (H_b - z)^{-2} (\mathbf{P}_A)_2 (H_b - z - \omega)^{-1} + (z \rightarrow z - w) \\ &\quad - \int_{\Gamma_{\omega}^1} dz z (\mathbf{P}_A)_1 (H_b - z)^{-1} (\mathbf{P}_A)_2 (H_b - z - \omega)^{-2} + (z \rightarrow z - w).\end{aligned}$$

Therefore, integrating by parts N times with respect to the complex variable z , one obtains 2^{N+1} terms, half of them is of the form

$$\int_{\Gamma_{\omega}^1} dz \frac{z^N}{N!} (\mathbf{P}_A)_1 (H_b - z)^{-N_1} (\mathbf{P}_A)_2 (H_b - z - \omega)^{-N_2} + (z \rightarrow z - w),$$

and the other half is of the form

$$\int_{\Gamma_{\omega}^1} dz \left(\mathcal{F}_{FD}^N(z) - \frac{z^N}{N!} \right) (\mathbf{P}_A)_1 (H_b - z)^{-N_1} (\mathbf{P}_A)_2 (H_b - z - \omega)^{-N_2} + (z \rightarrow z - w),$$

where $N_1, N_2 \in \mathbb{N}$ satisfy $N_1 + N_2 = N + 2$ and $1 \leq N_1, N_2 < N + 2$. Moreover, we have denoted by $\mathcal{F}_{FD}^N(z)$ the N -th exponentially decreasing antiderivative of $f_{FD}(z)$ and $(z \rightarrow z - w)$ means a term similar to the previous one but with z exchanged with $z - w$.

³The Fermi energy μ is defined by $\mu := \frac{E_+ - E_-}{2}$.

Similarly, one can integrate by parts the term defined by the complex integral on the open contour Γ_ω^2 . However, in this case one has to be more careful due to the contribution at infinity of the boundary terms. First, notice that the contour Γ_ω^2 is at finite distance from the spectrum of H_b , therefore Proposition A.1.1 implies that the norm of the operator $\Sigma(z, \omega)$ grows at most polynomial in $z \in \Gamma_\omega^2$ and (A.1.27), together with a Schur estimate implies, that the operator of the form $(\mathbf{P}_A)_i (H_b - z)^{-N_j}$ also have a norm that grows at most polynomially in $z \in \Gamma_\omega^2$. Furthermore, the antiderivatives of $f_{FD}(z)$ are exponentially decreasing as $\Re(z) \rightarrow +\infty$. This is sufficient to show that the boundary terms coming from the integration by parts vanishes. Then, the third operator reduces to a sum of terms of the form

$$\int_{\Gamma_\omega^2} dz \mathcal{F}_{FD}^N(z) (\mathbf{P}_A)_1 (H_b - z)^{-N_1} (\mathbf{P}_A)_2 (H_b - z - \omega)^{-N_2} + (z \rightarrow z - \omega).$$

In Section A.1 we prove that the operators of the type $(\mathbf{P}_A)_1 (H_b - z)^{-N_1}$ have a jointly continuous integral kernel and satisfy (A.1.27). Therefore, the three operators under the integral with respect to \underline{x} in (2.2.10), have a jointly continuous integral kernel. Moreover, because of that, we can separate the three operators and evaluate the integral and the limit $\beta \rightarrow \infty$ separately for each operator. Consider the third term after the integration by parts with respect to the complex variable z . For β large enough we have

$$\begin{aligned} & \left| \left(\int_{\Gamma_\omega^2} dz \mathcal{F}_{FD}^N(z) (\mathbf{P}_A)_1 (H_b - z)^{-N_1} (\mathbf{P}_A)_2 (H_b - z - \omega)^{-N_2} \right) (\underline{x}; \underline{x}') \right| \\ & \leq C \int_{\Gamma_\omega^2} dz \langle |z| \rangle^{10} e^{-\frac{\alpha}{r} \|\underline{x} - \underline{x}'\|} e^{-(\Re(z) - g)\beta} \leq C \int_{\Gamma_\omega^2} dz \langle |z| \rangle^{10} e^{-(\Re(z) - g)\alpha} \leq C, \end{aligned} \quad (2.2.11)$$

for some positive constants α and C , where in the first inequality we have used the estimate (A.1.27). From the estimate (2.2.11) it follows that we can exchange the integrals with the limit $\beta \rightarrow \infty$. Therefore, in view of $\lim_{\beta \rightarrow \infty} e^{-(\Re(z) - g)\beta} = 0$, the third term vanishes in the limit $\beta \rightarrow +\infty$. By mimicking this argument, the same can be proven for the second term.

Consider now the first term of (2.2.10). Performing the change of variable $z = z' - \frac{\omega}{2}$ in the first addendum of $\Sigma(z, \omega)$, and the change of variable $z = z' + \frac{\omega}{2}$ in the second addendum of $\Sigma(z, \omega)$, we can rewrite the first term of (2.2.10) as a complex integral around a suitable closed contour Γ that encloses only the spectral island contained in Γ_ω^1 such that $\Gamma \subset \rho(H + \omega)$ for $|\omega| < g$. Explicitly, we obtain

$$\begin{aligned} & \sigma(B, T = 0, \omega) \\ & = -\frac{1}{\pi\omega} \int_\Omega d\underline{x} \left[\int_\Gamma dz (\mathbf{P}_A)_1 \left(H_b - z + \frac{\omega}{2} \right)^{-1} (\mathbf{P}_A)_2 \left(H_b - z - \frac{\omega}{2} \right)^{-1} \right] (\underline{x}; \underline{x}). \end{aligned} \quad (2.2.12)$$

Because of the choice of Γ , the integrand in (2.2.12) is analytic in ω in a neighbourhood of the origin, therefore we can expand it in power series of ω . To simplify the notation, we drop for a while the subscript “ b ” of the Hamiltonian. By

expanding the resolvent we obtain

$$\begin{aligned} \sigma(B, T = 0, \omega) &= -\frac{1}{\pi} \int_{\Omega} d\mathbf{x} \left[\int_{\Gamma} dz \frac{1}{\omega} (\mathbf{P}_A)_1 (H - z)^{-1} (\mathbf{P}_A)_2 (H - z)^{-1} \right. \\ &+ \frac{1}{2} \int_{\Gamma} dz (\mathbf{P}_A)_1 (H - z)^{-1} (\mathbf{P}_A)_2 (H - z)^{-2} - (\mathbf{P}_A)_1 (H - z)^{-2} (\mathbf{P}_A)_2 (H - z)^{-1} \\ &\left. + \mathcal{O}(\omega) \right] (\underline{x}; \underline{x}). \end{aligned} \quad (2.2.13)$$

Notice that all the terms involved in the previous expression, (considering also the terms of order one in ω) are bounded. Apparently there is a first order pole in ω in the first term of (2.2.13). However, thanks to the presence of the complex contour integral, the integral kernel of the operator is zero along the diagonal, hence the pole does not contribute to the integral with respect to \underline{x} . Let us prove this claim. Consider

$$\left[(H - z)^{-1}, X_i \right] = i (H - z)^{-1} (\mathbf{P}_A)_i (H - z)^{-1}, \quad i = 1, 2, \quad (2.2.14)$$

where the commutator is initially well defined only on smooth functions. From (2.2.14) we get

$$\begin{aligned} &i \frac{1}{\pi} \int_{\Gamma} dz (\mathbf{P}_A)_1 (H - z)^{-1} (\mathbf{P}_A)_2 (H - z)^{-1} \\ &= i \frac{1}{\pi} \int_{\Gamma} dz (\mathbf{P}_A)_1 \left[(H - z)^{-1}, X_2 \right] \\ &= 2 [(\mathbf{P}_A)_1 \Pi_0, X_2]. \end{aligned}$$

Integrating by parts with respect to the complex variable z and using that the operator $(\mathbf{P}_A)_1 (H_b - z)^{-N}$ has a jointly continuous integral kernel for N large enough, it follows that $(\mathbf{P}_A)_1 \Pi_0$ has a smooth integral kernel. Therefore we get

$$(2 [(\mathbf{P}_A)_1 \Pi_0, X_2]) (\mathbf{x}; \mathbf{x}') = 2(x'_2 - x_2) ((\mathbf{P}_A)_1 \Pi_0) (\mathbf{x}; \mathbf{x}').$$

This shows that

$$-\frac{1}{\pi} \left(\int_{\Gamma} dz (\mathbf{P}_A)_1 (H - z)^{-1} (\mathbf{P}_A)_2 (H - z)^{-1} \right) (\underline{x}; \underline{x}) = 0.$$

Putting together all the previous results and taking the limit $\omega \rightarrow 0$ we obtain

$$\begin{aligned} &\sigma(b, T = 0, \omega = 0) \\ &= -\frac{1}{2\pi} \int_{\Omega} d\mathbf{x} \left[\int_{\Gamma} dz (\mathbf{P}_A)_1 (H - z)^{-1} (\mathbf{P}_A)_2 (H - z)^{-2} \right. \\ &\quad \left. - (\mathbf{P}_A)_1 (H - z)^{-2} (\mathbf{P}_A)_2 (H - z)^{-1} \right] (\underline{x}; \underline{x}) \end{aligned} \quad (2.2.15)$$

In the following we prove that the expression (2.2.15) for the conductivity is proportional to the Chern character of Π_0 .

Consider the definition of the Chern character rewritten using the Riesz projection (to simplify the notation we drop for a while also the superscript (b)):

$$\begin{aligned} \frac{C(\Pi_0)}{2\pi} &:= i\mathcal{T} \{ \Pi_0 [[\Pi_0, X_1], [\Pi_0, X_2]] \} \\ &= -\frac{i}{4\pi^2|\Omega|} \int_{\Omega} d\mathbf{x} \left\{ \Pi_0 \right. \\ &\quad \left. \oint_{\mathcal{C}_1} dz_1 \oint_{\mathcal{C}_2} dz_2 \left[[(H - z_1)^{-1}, X_1], [(H - z_2)^{-1}, X_2] \right] \Pi_0 \right\} (\mathbf{x}; \mathbf{x}), \end{aligned} \quad (2.2.16)$$

where we have chosen the positively oriented contours \mathcal{C}_1 and \mathcal{C}_2 such that they encircle the spectral island related to Π_0 and such that \mathcal{C}_1 is always strictly inside the area delimited by \mathcal{C}_2 . Let us start by studying the two contour integrals and considering only one term of the commutator. The other term will follow easily afterwards. Consider the following expression

$$[(H - z)^{-1}, X_i] = i(H - z)^{-1} (\mathbf{P}_A)_i (H - z)^{-1}, \quad i = 1, 2, \quad (2.2.17)$$

where the commutator is initially defined only on smooth functions and then extended by continuity to the whole Hilbert space. The first term of the commutator becomes

$$\begin{aligned} &-\oint_{\mathcal{C}_1} dz_1 \oint_{\mathcal{C}_2} dz_2 (H - z_1)^{-1} (\mathbf{P}_A)_1 (H - z_1)^{-1} \\ &\quad \cdot (H - z_2)^{-1} (\mathbf{P}_A)_2 (H - z_2)^{-1}. \end{aligned} \quad (2.2.18)$$

Since the contours \mathcal{C}_i are in the resolvent set of H_b , we can use the resolvent formula

$$(H - z_1)^{-1} (H - z_2)^{-1} = \frac{1}{z_1 - z_2} \left((H - z_1)^{-1} - (H - z_2)^{-1} \right). \quad (2.2.19)$$

By using the resolvent formula in (2.2.18), we obtain the sum of two terms defined by

$$\begin{aligned} A &:= -\Pi_0 \oint_{\mathcal{C}_1} dz_1 \oint_{\mathcal{C}_2} dz_2 \frac{1}{z_1 - z_2} (H - z_1)^{-1} (\mathbf{P}_A)_1 (H - z_1)^{-1} (\mathbf{P}_A)_2 (H - z_2)^{-1} \Pi_0, \\ B &:= \Pi_0 \oint_{\mathcal{C}_1} dz_1 \oint_{\mathcal{C}_2} dz_2 \frac{1}{z_1 - z_2} (H - z_1)^{-1} (\mathbf{P}_A)_1 (H - z_2)^{-1} (\mathbf{P}_A)_2 (H - z_2)^{-1} \Pi_0. \end{aligned}$$

Consider the first term A . Assuming that we can permute the terms under the complex integral, and using again the resolvent formula, we get the sum of others two terms

$$\begin{aligned} A_1 &:= \Pi_0 \oint_{\mathcal{C}_1} dz_1 \oint_{\mathcal{C}_2} dz_2 \frac{1}{(z_1 - z_2)^2} (\mathbf{P}_A)_1 (H - z_1)^{-1} (\mathbf{P}_A)_2 (H - z_2)^{-1} \Pi_0, \\ A_2 &:= -\Pi_0 \oint_{\mathcal{C}_1} dz_1 \oint_{\mathcal{C}_2} dz_2 \frac{1}{(z_1 - z_2)^2} (\mathbf{P}_A)_1 (H - z_1)^{-1} (\mathbf{P}_A)_2 (H - z_1)^{-1} \Pi_0. \end{aligned} \quad (2.2.20)$$

The proof of the cyclicity property is postponed to Section 2.2.2.

In A_1 we can perform the integration in z_1 . Since $\frac{1}{(z_1 - z_2)^2}$ is analytic in the interior of the area encircled by \mathcal{C}_1 , we can use Cauchy integral formula and after using the cyclicity property proved in Section 2.2.2, we obtain

$$-2\pi i \oint_{\mathcal{C}_2} dz_2 (\mathbf{P}_A)_1 \Pi_0 (H - z_2)^{-2} (\mathbf{P}_A)_2 (H - z_2)^{-1} \Pi_0. \quad (2.2.21)$$

Using the spectral representation of H we have that

$$\oint_{\mathcal{C}_2} dz_2 \int \int_{\lambda, \lambda' \in \sigma_0(H)} (\mathbf{P}_A)_1 (\lambda - z_2)^{-2} E^{(H)}(d\lambda) (\mathbf{P}_A)_2 (\lambda' - z_2)^{-1} E^{(H)}(d\lambda'),$$

where $E^{(H)}$ denote the spectral family of H . Notice that, for every $\lambda, \lambda' \in \sigma_0(H)$ it holds that

$$\oint_{\mathcal{C}_2} \frac{1}{(\lambda - z_2)^2} \frac{1}{(\lambda' - z_2)} dz_2 = 0, \quad (2.2.22)$$

by the residue theorem. Therefore, if it is possible to exchange the order of the two integrals, we can prove that $A_1 = 0$. The next lemma is devoted exactly to prove that we can actually exchange the order of the two integrals.

Lemma 2.2.3. *The expression in (2.2.21) is identically zero.*

Proof. Define $R(z) := (H - z)^{-1}$. Take $f, g \in C_0^\infty(\mathbb{R}^2)$ and consider the following scalar product

$$\begin{aligned} & \langle f, \oint_{\mathcal{C}_2} dz_2 (\mathbf{P}_A)_1 \Pi_0 R^2(z_2) (\mathbf{P}_A)_2 \Pi_0 R(z_2) \Pi_0 g \rangle \\ &= \langle f, \oint_{\mathcal{C}_2} dz_2 (\mathbf{P}_A)_1 R(i) \Pi_0 (H - i) \Pi_0 R^2(z_2) \\ & \quad \cdot (\mathbf{P}_A)_2 R^2(i) \Pi_0 R(z_2) \Pi_0 (H - i)^2 \Pi_0 g \rangle \quad (2.2.23) \\ &= \oint_{\mathcal{C}_2} dz_2 \langle f, (\mathbf{P}_A)_1 R^2(i) \Pi_0 (H - i)^2 \Pi_0 R^2(z_2) \\ & \quad \cdot (\mathbf{P}_A)_2 R^2(i) \Pi_0 R(z_2) \Pi_0 (H - i)^2 \Pi_0 g \rangle, \end{aligned}$$

where the last equality follows by recalling that $(\mathbf{P}_A)_1 R(i)$ and $(\mathbf{P}_A)_2 R(i)$ are bounded operators, and by the convergence in the uniform operator topology of the Riemann sums of the complex integral.

Then, for every $\epsilon > 0$, we introduce the regularizing operator $(e^{-\epsilon \langle X \rangle} f)(\mathbf{x}) = e^{-\epsilon \langle \mathbf{x} \rangle} f(\mathbf{x})$ for every $f \in L^2(\mathbb{R}^2)$. Considering the following limit in the operator norm

$$\begin{aligned} & \lim_{\epsilon \rightarrow 0} e^{-\epsilon \langle X \rangle} (\mathbf{P}_A)_2 R^2(i) \Pi_0 R(z_2) \Pi_0 (H - i)^2 \Pi_0 \\ &= (\mathbf{P}_A)_2 R^2(i) \Pi_0 R(z_2) \Pi_0 (H - i)^2 \Pi_0; \end{aligned}$$

we obtain that

$$\begin{aligned} & \lim_{\epsilon \rightarrow 0} \oint_{\mathcal{C}_2} dz_2 \langle f, (\mathbf{P}_A)_1 R(i) \Pi_0 (H - i) \Pi_0 R^2(z_2) e^{-\epsilon \langle X \rangle} (\mathbf{P}_A)_2 R^2(i) \\ & \quad \cdot \Pi_0 R(z_2) \Pi_0 (H - i)^2 \Pi_0 g \rangle \\ &= \langle f, \oint_{\mathcal{C}_2} dz_2 (\mathbf{P}_A)_1 R(i) \Pi_0 (H - i) \Pi_0 R^2(z_2) (\mathbf{P}_A)_2 R^2(i) \Pi_0 R(z_2) \Pi_0 (H - i)^2 \Pi_0 g \rangle \quad (2.2.24) \end{aligned}$$

where we have used the fact that the integrand is bounded and we are integrating on a bounded subset of \mathbb{C} . In order to prove that the right hand side of (2.2.24) is

zero, we show that for every ϵ the left hand side is zero. First of all consider the operator $A_\epsilon := e^{-\epsilon\langle X \rangle} (\mathbf{P}_A)_2 R^2(i)$. From

$$e^{-\epsilon\langle X \rangle} (\mathbf{P}_A)_2 R^2(i) = e^{-\epsilon\langle X \rangle} (-\Delta_A + i)^{-1} (-\Delta_A + i) (\mathbf{P}_A)_2 R^2(i) \quad (2.2.25)$$

it follows that A_ϵ is a compact operator. Indeed, $e^{-\epsilon\langle X \rangle} (-\Delta + i)^{-1}$ is a compact operator and together with Lemma 3.1.3 it implies that also $e^{-\epsilon\langle X \rangle} (-\Delta_A + i)^{-1}$ is compact operator. Moreover, $(-\Delta_A + i) (\mathbf{P}_A)_2 R^2(i)$ is a bounded operator. Hence A_ϵ is the limit in the uniform operator topology of finite rank operators, that is

$$\lim_{N \rightarrow \infty} T_N = A_\epsilon, \quad (2.2.26)$$

where $T_N := \sum_{j=1}^N |\tilde{f}_j\rangle\langle\tilde{g}_j|$ with $\tilde{f}_j, \tilde{g}_j \in L^2(\mathbb{R}^2)$. Therefore

$$\begin{aligned} & \langle f, \oint_{\mathcal{C}_2} dz_2 (\mathbf{P}_A)_1 R(i) \Pi_0 (H - i) \Pi_0 R^2(z_2) A_\epsilon \Pi_0 R(z_2) \Pi_0 (H - i)^2 \Pi_0 g \rangle \\ &= \langle f, \oint_{\mathcal{C}_2} dz_2 (\mathbf{P}_A)_1 R(i) \Pi_0 (H - i) \Pi_0 R^2(z_2) \lim_{N \rightarrow \infty} T_N \Pi_0 R(z_2) \Pi_0 (H - i)^2 \Pi_0 g \rangle \\ &= \lim_{N \rightarrow \infty} \sum_{j=1}^N \oint_{\mathcal{C}_2} dz_2 \langle f, (\mathbf{P}_A)_1 R(i) \Pi_0 (H - i) \Pi_0 R^2(z_2) \tilde{f}_j \rangle \\ & \quad \cdot \langle \tilde{g}_j, \Pi_0 R(z_2) \Pi_0 (H - i)^2 \Pi_0 g \rangle. \end{aligned} \quad (2.2.27)$$

Using now the spectral family of H_b , we obtain that the last expression is equal to

$$\oint_{\mathcal{C}_2} dz_2 \int \int_{\lambda, \lambda' \in \sigma_0(H)} (\lambda - z_2)^{-2} (\lambda' - z_2)^{-1} \langle Cf, E^{(H)}(d\lambda) \tilde{f}_j \rangle \langle D\tilde{g}_j, E^{(H)}(d\lambda') g \rangle. \quad (2.2.28)$$

where C and D are bounded operators. Therefore we can apply Fubini's theorem and exchange the order of the three integrals. Since the integral in z_2 vanishes, we have proved that the expression in (2.2.23) is zero for every $f, g \in C_0^\infty(\mathbb{R}^2)$. A standard density argument concludes the proof. \square

The second term, A_2 , is zero simply integrating in z_2 . Indeed the function $(z_2 - z_1)^{-2}$ admits an antiderivative and we are integrating along a closed contour.

Consider now the term B . Even in this case, assuming again that we can permute the term under the complex integral, and using again the resolvent formula, we obtain two terms

$$\begin{aligned} B_1 + B_2 &:= -\Pi_0 \oint_{\mathcal{C}_1} dz_1 \oint_{\mathcal{C}_2} dz_2 \frac{1}{(z_1 - z_2)^2} (\mathbf{P}_A)_1 (H - z_2)^{-1} (\mathbf{P}_A)_2 (H - z_2)^{-1} \Pi_0 \\ & \quad + \Pi_0 \oint_{\mathcal{C}_1} dz_1 \oint_{\mathcal{C}_2} dz_2 \frac{1}{(z_1 - z_2)^2} (\mathbf{P}_A)_1 (H - z_2)^{-1} (\mathbf{P}_A)_2 (H - z_1)^{-1} \Pi_0. \end{aligned} \quad (2.2.29)$$

The first term B_1 is zero for the same reason of A_2 , then it remains only B_2 . By performing the integration in z_1 we obtain

$$-2\pi i \Pi_0 \oint_{\mathcal{C}_2} dz_2 (\mathbf{P}_A)_1 (H - z_2)^{-1} (\mathbf{P}_A)_2 (H - z_2)^{-2} \Pi_0.$$

Eventually, considering also the second term of the commutator, we obtain that the expression for $C(\Pi_0)$ is equal to :

$$-\frac{1}{2\pi} \int_{\Omega} d\underline{x} \left[\Pi_0 \oint_{\mathcal{C}_2} dz_2 (\mathbf{P}_A)_1 (H - z_2)^{-1} (\mathbf{P}_A)_2 (H - z_2)^{-2} \Pi_0 \right. \\ \left. - \Pi_0 \oint_{\mathcal{C}_2} dz_2 (\mathbf{P}_A)_2 (H - z_2)^{-1} (\mathbf{P}_A)_1 (H - z_2)^{-2} \Pi_0 \right] (\underline{x}; \underline{x}). \quad (2.2.30)$$

A direct comparison with formula (2.2.15) is not successful, in particular the expression (2.2.30) is the same of the one in (2.2.15) apart from the two Π_0 under the integral with respect to \underline{x} . Therefore we proceed in the following way. Since Π_0 is a projection, it squares to itself, hence instead of calculating the derivative of $\mathcal{I}(\Pi_0)$, we consider the derivative of $\mathcal{I}(\Pi_0^2)$. We start by calculating $(\Pi_0^{(b+\epsilon)})^2$.

In order to compute the first derivative, we expand $(\Pi_0^{(b+\epsilon)})^2$ in power of ϵ and consider only the first order terms. First of all consider that the gaps in the spectrum of H_b are stable against small variations of the magnetic field [85], therefore, from the magnetic perturbation theory [87], we get the following expansion

$$\begin{aligned} \Pi_0^{(b+\epsilon)}(\mathbf{x}; \mathbf{y}) &= e^{i\epsilon\phi(\mathbf{x}, \mathbf{y})} \Pi_0^{(b)}(\mathbf{x}; \mathbf{y}) \\ &=: e^{i\epsilon\phi(\mathbf{x}, \mathbf{y})} \Pi_0^{(b)}(\mathbf{x}; \mathbf{y}) + \epsilon e^{i\epsilon\phi(\mathbf{x}, \mathbf{y})} W(\mathbf{x}; \mathbf{y}) + \mathcal{O}(\epsilon^2). \end{aligned} \quad (2.2.31)$$

Where $W(\mathbf{x}; \mathbf{y})$ is given by

$$W(\mathbf{x}; \mathbf{y}) = \frac{i}{2\pi} \oint_{\mathcal{C}_2} \left\{ \int_{\mathbb{R}^2} d\mathbf{x}' (H_b - z)^{-1}(\mathbf{x}; \mathbf{x}') S(\mathbf{x}' - \mathbf{y}) (H_b - z)^{-1}(\mathbf{x}'; \mathbf{y}) \right\} dz, \quad (2.2.32)$$

with $S(\mathbf{x}' - \mathbf{y}) = (\mathbf{P}_A)_{\mathbf{x}'} \cdot A(\mathbf{x}' - \mathbf{y})$, where the notation $(\mathbf{P}_A)_{\mathbf{x}'}$ means that the operator (\mathbf{P}_A) acts only on the variable \mathbf{x}' . Taking into account the explicit formula (2.2.31), the integral kernel of $(\Pi_0^{(b+\epsilon)})^2$ is given by

$$\begin{aligned} (\Pi_0^{(b+\epsilon)})^2(\mathbf{x}; \mathbf{y}) &= e^{i\epsilon\phi(\mathbf{x}, \mathbf{y})} \Pi_0^{(b)}(\mathbf{x}; \mathbf{y}) \\ &+ \epsilon \int_{\mathbb{R}^2} d\mathbf{x}' e^{i\epsilon\phi(\mathbf{x}, \mathbf{x}')} \Pi_0^{(b)}(\mathbf{x}; \mathbf{x}') e^{i\epsilon\phi(\mathbf{x}', \mathbf{y})} W(\mathbf{x}'; \mathbf{y}) \\ &+ \epsilon \int_{\mathbb{R}^2} d\mathbf{x}' e^{i\epsilon\phi(\mathbf{x}, \mathbf{x}')} W(\mathbf{x}; \mathbf{x}') e^{i\epsilon\phi(\mathbf{x}', \mathbf{y})} \Pi_0^{(b)}(\mathbf{x}'; \mathbf{y}) \\ &+ \mathcal{O}(\epsilon^2). \end{aligned} \quad (2.2.33)$$

Notice that the terms of order ϵ^2 are bounded due to exponential localization of the integral kernel of Π_0 . Since we have to compute the trace of $(\Pi_0^{(b+\epsilon)})^2$, we are interested only in the diagonal elements of the integral kernel, namely

$$\begin{aligned} (\Pi_0^{(b+\epsilon)})^2(\mathbf{x}; \mathbf{x}) &= \Pi_0^{(b)}(\mathbf{x}; \mathbf{x}) + \epsilon \int_{\mathbb{R}^2} d\mathbf{x}' \Pi_0^{(b)}(\mathbf{x}; \mathbf{x}') W(\mathbf{x}', \mathbf{y}) + W(\mathbf{x}; \mathbf{x}') \Pi_0^{(b)}(\mathbf{x}'; \mathbf{x}) \\ &+ \mathcal{O}(\epsilon^2) \end{aligned}$$

where we have used $\phi(\mathbf{x}, \mathbf{x}') + \phi(\mathbf{x}', \mathbf{x}) = 0$. Hence, the derivative with respect to b of the integrated density of states is given by

$$\frac{2}{|\Omega|} \int_{\Omega} d\underline{x} \{ \Pi_0 W \} (\underline{x}; \underline{x}), \quad (2.2.34)$$

where we have used the cyclicity property.

Consider now the integral kernel $W(\mathbf{x}, \mathbf{y})$. From equation (2.2.17) and $\mathbf{A}(\mathbf{x}) = \frac{1}{2}(-\mathbf{x}_2, \mathbf{x}_1)$ we obtain that

$$\mathbf{A}(\mathbf{x}' - \mathbf{y}) (H_b - z)^{-1}(\mathbf{x}'; \mathbf{y}) = -\frac{i}{2} \mathbf{e}_3 \wedge \left[(H_b - z)^{-1} \mathbf{P}_A (H_b - z)^{-1} \right](\mathbf{x}'; \mathbf{y}),$$

where $\mathbf{e}_3 := (0, 0, 1)$. Therefore, substituting the last expression in (2.2.32) we get

$$\begin{aligned} \frac{d\mathcal{I}(\Pi_0^{(b)})}{db} &= \frac{d\mathcal{I}\left(\left(\Pi_0^{(b)}\right)^2\right)}{db} \\ &= -\frac{1}{2\pi} \int_{\Omega} d\mathbf{x} \left[\Pi_0^{(b)} \oint_{\mathcal{C}_2} dz_2 (H_b - z_2)^{-1} (\mathbf{P}_A)_1 (H_b - z_2)^{-1} (\mathbf{P}_A)_2 (H_b - z_2)^{-1} \Pi_0^{(b)} \right. \\ &\quad \left. - \Pi_0^{(b)} \oint_{\mathcal{C}_2} dz_2 (H_b - z_2)^{-1} (\mathbf{P}_A)_2 (H_b - z_2)^{-1} (\mathbf{P}_A)_1 (H_b - z_2)^{-1} \Pi_0^{(b)} \right](\underline{x}; \underline{x}). \end{aligned}$$

Hence we obtain that

$$\left. \frac{d\mathcal{I}(\Pi_0^{(b)})}{db} \right|_{b=b_0} = \frac{C(\Pi_0^{(b_0)})}{2\pi}. \quad (2.2.35)$$

Considering $\Pi_0^{(b)}$, instead of $(\Pi_0^{(b)})^2$, and repeating the same argument (see [38] for the explicit computation) one also obtains that

$$\frac{C(\Pi_0^{(b)})}{2\pi} = \sigma(b_0, T = 0, \omega = 0). \quad (2.2.36)$$

Therefore the proof of Theorem 2.2.1 is concluded.

Remark 2.2.4. The Středa formula, as it was showed in [110] by Středa, is given by equation (2.2.35). Instead, equation (2.2.36) goes under the name of gap labelling theorem. The proof we have shown for equation (2.2.36) is not particularly illuminating, in fact it follows the inverse logical path: we started from the definition of the Chern character and we proved that it is equal to the derivative of the integrated density of states. In Section 2.4 we provide a simpler and more elegant proof of the gap labelling theorem starting from the integrated density of states and showing directly that the first order contribution in ϵ to the integrated density of states $\mathcal{I}(\Pi_0^{(b+\epsilon)})$ is given by the formula of the Chern character given in Definition 2.1.3.

2.2.2 Integral kernels and cyclicity

This section is devoted to the proof of cyclicity under the trace per unit volume when the operators involved have jointly continuous integral kernel. Let us recall the underlining idea from [38]. Consider two operators K_1 and K_2 with jointly continuous integral kernels such that, for all $\mathbf{x}, \mathbf{y} \in \mathbb{R}^2$,

$$K_i(\mathbf{x}; \mathbf{y}) = K_i(\mathbf{x} + \gamma; \mathbf{y} + \gamma), \quad \forall \gamma \in \mathbb{Z}^2, \quad i \in 1, 2,$$

we are interested in evaluating the trace per unit volume, see Remark 2.1.2, given by

$$\mathcal{T}(K_1 K_2) = \int_{\Omega} d\mathbf{x} \int_{\mathbb{R}^2} d\mathbf{y} K_1(\underline{x}; \mathbf{y}) K_2(\mathbf{y}; \underline{x}).$$

Then, from the translation invariance of the kernel we obtain

$$\begin{aligned}
\int_{\Omega} d\mathbf{x} \int_{\mathbb{R}^2} d\mathbf{y} K_1(\mathbf{x}; \mathbf{y}) K_2(\mathbf{y}; \mathbf{x}) &= \sum_{\gamma \in \mathbb{Z}^2} \int_{\Omega} d\mathbf{x} \int_{\Omega} d\mathbf{y} K_1(\mathbf{x}; \mathbf{y} + \gamma) K_2(\mathbf{y} + \gamma; \mathbf{x}) \\
&= \sum_{\gamma \in \mathbb{Z}^2} \int_{\Omega} d\mathbf{x} \int_{\Omega} d\mathbf{y} K_1(\mathbf{x} - \gamma; \mathbf{y}) K_2(\mathbf{y}; \mathbf{x} - \gamma) \\
&= \int_{\Omega} d\mathbf{y} \int_{\mathbb{R}^2} d\mathbf{x} K_2(\mathbf{y}; \mathbf{x}) K_1(\mathbf{x}; \mathbf{y}) = \mathcal{T}(K_2 K_1),
\end{aligned} \tag{2.2.37}$$

which shows that we can cycle the operators under the trace per unit volume. Note that this result in general is not obvious, since it would require to know some properties regarding the commutator between K_i and χ_L . We want to use the previous argument in order to show that, for $m \in \{0, 1\}$,

$$\begin{aligned}
&\mathcal{T} \left(\Pi_0^m \oint_{\mathcal{C}} dz (H_b - z)^{-1} (\mathbf{P}_A)_i (H_b - z)^{-1} (\mathbf{P}_A)_j (H_b - z)^{-1} \Pi_0^m \right) \\
&= \mathcal{T} \left(\Pi_0^m \oint_{\mathcal{C}} dz (\mathbf{P}_A)_i (H_b - z)^{-1} (\mathbf{P}_A)_j (H_b - z)^{-2} \Pi_0^m \right).
\end{aligned} \tag{2.2.38}$$

Hence we have to write the operator under the trace as a product of two operators with jointly continuous integral kernel such that their diagonal elements are translation invariant. Let us show this in details. By integrating by part N times on the closed contour \mathcal{C} we obtain a sum of terms of the form

$$\oint_{\mathcal{C}} dz \frac{z^N}{N!} (H_b - z)^{-N_1} (\mathbf{P}_A)_i (H_b - z)^{-N_2} (\mathbf{P}_A)_j (H_b - z)^{-N_3},$$

where $N_1, N_2, N_3 \in \mathbb{N}$ satisfy $N_1 + N_2 + N_3 = N + 3$ and $1 \leq N_1, N_2, N_3 < N + 3$. In Section A.1 we show that, for $M > 0$ large enough, the operators of the form $(H_b - z)^{-M}$ and $(\mathbf{P}_A)_j (H_b - z)^{-M}$ have a jointly continuous integral kernel that grows at most polynomially in the complex variable z and is exponentially localized near the diagonal, see (A.1.23) and (A.1.27). Therefore, the operators $K_1 := \Pi_0^m (H_b - z)^{-N_1} (\mathbf{P}_A)_i (H_b - z)^{-N_2}$ and $K_2 := (\mathbf{P}_A)_j (H_b - z)^{-N_3} \Pi_0^m$ have a jointly continuous integral kernel and the traces per unit volume in (2.2.38) make sense. In view of the boundedness of the contour \mathcal{C} , in order to apply the cyclicity argument showed in (2.2.37), it remains only to check that the diagonal elements of their integral kernels are translation invariant. Since both $(H_b - z)^{-1}$ and \mathbf{P}_A commute with the magnetic translations, their integral kernels satisfy

$$K_i(\mathbf{x}; \mathbf{y}) = e^{i\phi(\mathbf{x}, \gamma)} K_i(\mathbf{x} - \gamma; \mathbf{y} - \gamma) e^{-i\phi(\mathbf{x}', \gamma)} \quad \mathbf{x}, \mathbf{x}' \in \mathbb{R}^2, \gamma \in \mathbb{Z}^2.$$

Therefore we have that $K_i(\mathbf{x}; \mathbf{y}) = K_i(\mathbf{x} - \gamma; \mathbf{y} - \gamma)$ and we can freely apply the cyclicity argument in the proof of the previous section.

2.3 Time-reversal symmetry always implies zero Chern character

In time-reversal symmetric systems, it is the existence of the time-reversal symmetry operator Θ that implies the vanishing of the Chern number of the Fermi projection.

Indeed, by plugging the relation

$$\Theta \Pi_0(\mathbf{k}) \Theta^{-1} = \Pi_0(-\mathbf{k})$$

in the definition of the Chern number (5.3.2) the previous claim can be easily proved, see also [89]. The question we want to answer is whether this property requires the existence of an underlining periodic structure, or rather it is sufficient to have a time-reversal symmetric system.

Consider a Hamiltonian operator H that satisfies Assumption 1.3.3. Assume that the Hamiltonian is time-reversal symmetric, that is assume that the magnetic vector potential $\mathbf{A} = 0$ so that the Hamiltonian is a real operator. Therefore, consider the projection Π_0 onto the isolated spectral island of H . By the holomorphic functional calculus, also Π_0 is a real operator. Since we know from Section A.1 that Π_0 has a jointly continuous integral kernel, as a real and selfadjoint operator its integral kernel satisfies

$$\Pi_0(\mathbf{x}; \mathbf{y}) = \Pi_0(\mathbf{y}; \mathbf{x}), \quad \forall \mathbf{x}, \mathbf{y} \in \mathbb{R}^2.$$

This means that $\Pi_0 = \Pi_0^\top$, where we denoted with $^\top$ the operator whose integral kernel coordinates are switched. The Chern character of Π_0 is given by

$$C(\Pi_0) = \lim_{L \rightarrow \infty} \frac{2\pi}{4L^2} \text{Tr} (i\chi_L \Pi_0 [[X_1, \Pi_0], [X_2, \Pi_0]] \Pi_0 \chi_L) =: \lim_{L \rightarrow \infty} \frac{2\pi}{4L^2} \text{Tr} (\mathfrak{C}_L),$$

compare with Definition 2.1.3. In Chapter 4 we prove that \mathfrak{C}_L is a trace class operator for every L , hence the previous formula is well defined whenever the limit on the right hand side exists. From the joint continuity of the integral kernel of Π_0 and from the identity

$$[X_i, \Pi_0](\mathbf{x}; \mathbf{y}) = (\mathbf{x} - \mathbf{y}) \Pi_0(\mathbf{x}; \mathbf{y}), \quad \forall \mathbf{x}, \mathbf{y} \in \mathbb{R}^2,$$

one can easily deduce that the integral kernel of \mathfrak{C}_L is also jointly continuous. The action of switching the variables of the integral kernel of bounded linear operator is the infinite dimensional analogue of the transposition operation on matrices. Indeed, if A is a trace class operator with jointly continuous integral kernel it holds that

$$\text{Tr}(A) = \int_{\mathbb{R}^2} d\mathbf{x} A(\mathbf{x}; \mathbf{x}),$$

which implies $\text{Tr}(A) = \text{Tr}(A^\top)$. Moreover, if B and C are trace class operators with jointly continuous integral kernel we have that

$$\begin{aligned} (BC)^\top(\mathbf{x}; \mathbf{y}) &= \int_{\mathbb{R}^2} d\mathbf{x}' B(\mathbf{y}; \mathbf{x}') C(\mathbf{x}'; \mathbf{x}) \\ &= \int_{\mathbb{R}^2} d\mathbf{x}' C^\top(\mathbf{x}; \mathbf{x}') B^\top(\mathbf{x}'; \mathbf{y}) = C^\top B^\top(\mathbf{x}; \mathbf{y}), \end{aligned}$$

which implies

$$[B, C]^\top(\mathbf{x}; \mathbf{y}) = [C^\top, B^\top](\mathbf{x}; \mathbf{y}). \quad (2.3.1)$$

Applying these two properties to $\text{Tr}(\mathfrak{C}_L)$, we have the following chain of equalities

$$\begin{aligned} \text{Tr}(\mathfrak{C}_L) &= \text{Tr}(\mathfrak{C}_L^\top) = \text{Tr} \left\{ i(\chi_L \Pi_0 [[X_1, \Pi_0], [X_2, \Pi_0]] \Pi_0 \chi_L)^\top \right\} \\ &= \text{Tr} \left\{ i(\Pi_0 \chi_L)^\top [[X_2, \Pi_0]^\top, [X_1, P]^\top] (\chi_L \Pi_0)^\top \right\}. \end{aligned} \quad (2.3.2)$$

Consider the operator $\Pi_0\chi_L$, it has a jointly continuous integral kernel given by

$$\Pi_0\chi_L(\mathbf{x}; \mathbf{y}) = \Pi_0(\mathbf{x}; \mathbf{y})\chi_L(\mathbf{y}),$$

hence we have that

$$(\Pi_0\chi_L)^\top(\mathbf{x}; \mathbf{y}) = \Pi_0(\mathbf{y}; \mathbf{x})\chi_L(\mathbf{x}) = \Pi_0(\mathbf{x}; \mathbf{y})\chi_L(\mathbf{x}) = (\chi_L\Pi_0)(\mathbf{x}; \mathbf{y}), \quad (2.3.3)$$

where in the second equality we have used the time-reversal symmetry of Π_0 . Consider now the commutators $[X_i, \Pi_0]$

$$\begin{aligned} [X_i, \Pi_0]^\top(\mathbf{x}; \mathbf{y}) &= [X_i, \Pi_0](\mathbf{y}; \mathbf{x}) = (\mathbf{y}_i - \mathbf{x}_i)\Pi_0(\mathbf{y}; \mathbf{x}) \\ &= (\mathbf{y}_i - \mathbf{x}_i)\Pi_0(\mathbf{x}; \mathbf{y}) = -[X_i, \Pi_0](\mathbf{x}; \mathbf{y}), \end{aligned} \quad (2.3.4)$$

where again in the third equality we have used the time-reversal symmetry of Π_0 . Plugging (2.3.3) and (2.3.4) in (2.3.2), we obtain

$$\mathrm{Tr} \{i\chi_L\Pi_0 [[X_2, \Pi_0], [X_1, P]] \Pi_0\chi_L\} = -\mathrm{Tr} \{i\chi_L\Pi_0 [[X_1, P], [X_2, \Pi_0]] \Pi_0\chi_L\}.$$

Therefore we have that $\mathrm{Tr}(\mathfrak{C}_L) = -\mathrm{Tr}(\mathfrak{C}_L)$ and this implies $\mathrm{Tr}(\mathfrak{C}_L) = 0$ which in turn implies $C(\Pi_0) = 0$.

The above argument shows that the vanishing of the Chern character for time-reversal symmetric systems does not depend on the \mathbf{k} -space structure of periodic systems.

2.4 Beyond Diophantine Wannier diagram: gap labelling for Bloch–Landau Hamiltonian

In this section we analyse the relations between the Chern character and the integrated density of states, in particular we provide a new proof of the gap labelling theorem for Bloch–Landau Hamiltonian. As a by-product we show that the Chern character is stable with respect to perturbation by a constant magnetic field. This section is the reproduction of [32] which is the fruit of a joint collaboration with H. Cornean and D. Monaco.

It is well known that, given a two-dimensional purely magnetic Landau Hamiltonian with a constant magnetic field b which generates a magnetic flux φ per unit area, then any spectral island σ_b consisting of M infinitely degenerate Landau levels carries an integrated density of states $\mathcal{I}_b = M\varphi$. Wannier later discovered a similar Diophantine relation expressing the integrated density of states of a gapped group of bands of the Hofstadter Hamiltonian as a linear function of the magnetic field flux with integer slope.

We extend this result to a gap labelling theorem for any two-dimensional Bloch–Landau operator H_b which also has a bounded \mathbb{Z}^2 -periodic electric potential. Assume that H_b has a spectral island σ_b which remains isolated from the rest of the spectrum as long as φ lies in a compact interval $[\varphi_1, \varphi_2]$. Then $\mathcal{I}_b = c_0 + c_1\varphi$ on such intervals, where the constant $c_0 \in \mathbb{Q}$ while $c_1 \in \mathbb{Z}$. The integer c_1 is the Chern character of the spectral projection onto the spectral island σ_b . We also show that, as a Corollary

of the main result, the Fermi projection on σ_b , albeit continuous in b in the strong topology, is nowhere continuous in the norm topology if either $c_1 \neq 0$ or $c_1 = 0$ and φ is rational.

Our proofs, otherwise elementary, do not use non-commutative geometry but are based on gauge covariant magnetic perturbation theory which we briefly review for the sake of the reader. Moreover, our method allows us to extend the analysis to certain non-covariant systems having slowly varying magnetic fields.

2.4.1 Introduction and main results

It is by now textbook material [72, 93] that each Landau level of an electron moving freely in two dimensions in the presence of a constant magnetic field \mathbf{B} carries a density of states per unit area equal to the magnetic field flux $\varphi = \frac{\mathbf{B}}{2\pi c}$, in Hartree units where $e = 1 = m_e = \hbar$.

In 1978, Wannier [114] realized by an ingenious counting argument that the integrated density of states of any isolated group of mini-bands of the Hofstadter Hamiltonian [62], a discrete analogue of the magnetic Laplacian, is a linear Diophantine function of the rational magnetic flux. Moreover, its slope is an integer which remains unchanged as long as the group of mini-bands under consideration remains isolated from the other ones. More specifically, if $\mathcal{I}_{\mathbf{B}_0}$ denotes the integrated density of states associated to M mini-bands of the Hofstadter Hamiltonian at magnetic field \mathbf{B}_0 such that $\mathbf{B}_0 = 2\pi c p/q$, with $p, q \in \mathbb{Z}$ co-prime integers, then

$$q\mathcal{I}_{\mathbf{B}_0} = M + c_1 p, \quad c_1 \in \mathbb{Z}. \quad (2.4.1)$$

Notice that the left-hand side of the above equality counts the number of charge carriers in a supercell of area q . Without giving a formal proof, Wannier came to the natural conclusion that this relationship should also hold for all irrational values of the flux: this allowed him to label the gaps in the spectrum of the Hofstadter Hamiltonian by “diagrams” consisting of linear functions of magnetic flux with integer slopes. No wonder that his paper was rather cryptically entitled *A Result Not Dependent on Rationality for Bloch Electrons in a Magnetic Field*.

In 1982, starting from the linear response ansatz, Středa [110] showed that the Hall conductivity is proportional to the derivative with respect to the magnetic flux of the integrated density of states of the Fermi projection, provided the Fermi energy is in a gap. Then in [109] he used Wannier’s result from 1978 in order to conclude that the Hall conductivity is proportional to an integer, namely c_1 in the above formula (2.4.1).

Still in 1982, Thouless, Kohomoto, Nightingale and den Nijs [112] showed that the Hall conductivity is proportional to the Chern number of the Fermi projection whenever the number of magnetic flux quanta per unit cell is rational, and thus identified the geometric origin underlying the integer c_1 : this relation of the Hall conductivity with topological numbers was later clarified by Avron, Seiler and Simon, see [8]. Reasoning in analogy with the Hofstadter model, and inspired by Wannier’s work, Thouless and his collaborators concluded that the results should persist also at irrational values of the magnetic flux. This led Avron and Osadchy to produce “colored Hofstadter butterflies”, where the gaps in the spectrum of the Hofstadter Hamiltonian are labelled according to their associated Chern number [88, 6].

For discrete and continuous gapped models of Bloch electrons, Wannier’s result and its connection with the Chern character for all real flux values were rigorously formulated by Bellissard [12, 13] in the language of non-commutative geometry. The equality argued by Wannier, generalizing (2.4.1) to any b , was dubbed “gap labelling conjecture” in [12], and translated in a statement about the K -theory of certain crossed product C^* -algebras. Bellissard proved the gap labelling conjecture for aperiodic crystals without magnetic field in [14]; the full proof of the “magnetic” gap labelling conjecture was achieved by Benameur and Mathai in [16, 17]. In the case of periodic potentials, the proof of the K -theoretic reformulation of the magnetic gap labelling conjecture can be traced back to a theorem by Elliott [44] on the K -theory of the rotation C^* -algebra, elaborating upon earlier results by Connes [27], Pimsner and Voiculescu [94], and Rieffel [101] for the two-dimensional case which is also of interest for the work presented in this section. Unfortunately, Bellissard used the term “Středa formula” to denote the equality between the derivative of the integrated density of states and the Chern character, although Středa’s contribution strictly consisted in relating the derivative with respect to the magnetic field of the integrated density of states with the Hall conductivity, within linear response. We note that the actual “Středa formula”, in the latter sense, was rigorously proved in the gapped continuous case by Cornean, Nenciu and Pedersen in [38], in Section 2.2.1 we reported the proof with the detailed steps.

Schulz-Baldes and Teufel [102] significantly improved the results of Středa and also extended the results of [13] to the case when the Fermi energy is situated in a mobility gap (see also [15] for the proof of integrality of the Chern character in the latter regime). Of a similar flavour are certain higher-dimensional generalizations of the “Středa formula”, presented in the monograph by Prodan and Schulz-Baldes [97]. We note though that their proofs are formulated for bounded Hamiltonian operators.

Goals and structure

In this section, we first provide a proof of the Wannier diagrams for unbounded continuous Bloch–Landau Hamiltonians; we achieve this in Theorem 2.4.1 (i) and (ii). As a by-product, we show in Corollary 2.4.2 that while the Fermi projection is always everywhere continuous in the strong topology as a function of the magnetic flux, there are situations in which this map is nowhere continuous in the norm topology!

Our second novel result, Theorem 2.4.5, extends the gap labelling (in a weaker sense) to more general perturbations; in particular, we are interested in perturbations given by slowly varying magnetic fields, which generically break covariance.

The main tool we use is the so-called gauge covariant magnetic perturbation theory developed by Cornean and Nenciu [36, 87, 37, 29]. We do not use noncommutative geometry, and clarify the physical meaning of the “gap labelling” through Wannier diagrams.

In the rest of this section we formulate our two main result, namely Theorem 2.4.1 and Theorem 2.4.5. In Section 2.4.2 we prove Theorem 2.4.1, in Section 2.4.4 we prove Theorem 2.4.5, while in Appendix 2.5.1 we review the magnetic Bloch–Floquet transform and the Chern number. We end with Appendix 2.5.2 in which we review the gauge covariant magnetic perturbation theory.

The covariant setting

We consider a Bloch–Landau Hamiltonian acting on $L^2(\mathbb{R}^2)$, and defined in Hartree units by

$$H_b = \frac{1}{2} (\mathbf{P} - b\mathbf{A})^2 + V,$$

where $\mathbf{P} = -i\nabla$ is the usual momentum operator, $b = -\frac{1}{c}\mathbf{B} \in \mathbb{R}$ and \mathbf{B} is the magnetic field strength, $\mathbf{A} = \frac{1}{2}(-x_2, x_1)$ is the magnetic potential in the symmetric gauge. V is a \mathbb{Z}^2 -periodic electric potential; although we could handle certain singularities, in order to streamline the proofs we choose to work with bounded V 's. Under these conditions, H_b is essentially selfadjoint on $C_0^\infty(\mathbb{R}^2)$.

Suppose that the spectrum of H_b has an isolated spectral island σ_b ; by definition, isolated means that it is separated by the rest of the spectrum by one or two gaps. The edges of these gaps vary continuously with b [85], thus via the Riesz formula we can define the spectral projection

$$\Pi_b = \frac{i}{2\pi} \oint_{\mathcal{C}} (H_b - z)^{-1} dz$$

where \mathcal{C} is a positively oriented simple contour encircling σ_b and staying at a positive distance from the spectrum as long as the two gaps we started with remain open. We note that the nature and the structure of σ_b can dramatically change when b varies, i.e. internal mini-gaps can open or close, but as a set, σ_b varies continuously with respect to the Hausdorff distance. It is possible to prove that Π_b admits a jointly continuous integral kernel, see Appendix 2.5.2. Using Combes–Thomas estimates [26, 37] (see also Appendix 2.5.2) one can prove the existence of $\alpha, C > 0$ such that

$$|\Pi_b(\mathbf{x}; \mathbf{x}')| \leq C e^{-\alpha\|\mathbf{x}-\mathbf{x}'\|}, \quad \forall \mathbf{x}, \mathbf{x}' \in \mathbb{R}^2. \quad (2.4.2)$$

These two constants can be chosen uniformly in b as long as b varies in an interval such that σ_b is well separated from the rest of the spectrum.

Let Λ_L be the square of side-length $L > 1$ centred at the origin and let χ_L be its characteristic function. Due to (2.4.2) we have that both $\chi_L \Pi_b e^{\alpha\|\cdot\|/2}$ and $e^{-\alpha\|\cdot\|/2} \Pi_b$ are Hilbert–Schmidt operators, thus

$$\chi_L \Pi_b = \left\{ \chi_L \Pi_b e^{\alpha\|\cdot\|/2} \right\} \left\{ e^{-\alpha\|\cdot\|/2} \Pi_b \right\} \quad (2.4.3)$$

is trace class with $\text{Tr}(|\chi_L \Pi_b|) \leq C L^2$.

In the above considerations, the periodicity of V played no role. When V is \mathbb{Z}^2 -periodic, we decompose every point $\mathbf{x} \in \mathbb{R}^2$ uniquely as

$$\mathbf{x} = \gamma + \underline{x}, \quad \gamma \in \mathbb{Z}^2, \quad \underline{x} \in (-1/2, 1/2] \times (-1/2, 1/2] =: \Omega.$$

Define the Peierls antisymmetric phase by

$$\phi(\mathbf{x}, \mathbf{x}') := \frac{1}{2}(x'_1 x_2 - x'_2 x_1), \quad \forall \mathbf{x}, \mathbf{x}' \in \mathbb{R}^2. \quad (2.4.4)$$

The phase satisfies the composition rule

$$\phi(\mathbf{x}, \mathbf{y}) + \phi(\mathbf{y}, \mathbf{x}') = \phi(\mathbf{x}, \mathbf{x}') + \phi(\mathbf{x} - \mathbf{y}, \mathbf{y} - \mathbf{x}') \quad \forall \mathbf{x}, \mathbf{y}, \mathbf{x}' \in \mathbb{R}^2. \quad (2.4.5)$$

The Hamiltonian H_b commutes with the magnetic translations $\tau_{b,\eta}$, defined for every $\eta \in \mathbb{Z}^2$ by

$$(\tau_{b,\eta}\psi)(\mathbf{x}) := e^{ib\phi(\mathbf{x},\eta)}\psi(\mathbf{x} - \eta), \quad \forall \psi \in L^2(\mathbb{R}^2).$$

Because Π_b then also commutes with the magnetic translations, for every $\eta \in \mathbb{Z}^2$ we have

$$\Pi_b(\mathbf{x}; \mathbf{x}') = e^{ib\phi(\mathbf{x},\eta)}\Pi_b(\mathbf{x} - \eta; \mathbf{x}' - \eta)e^{-ib\phi(\mathbf{x}',\eta)}. \quad (2.4.6)$$

We can then define the integrated density of states for the projection $\mathcal{I}(\Pi_b)$ by the formula

$$\mathcal{I}(\Pi_b) := \lim_{L \rightarrow \infty} \frac{1}{|\Lambda_L|} \text{Tr}(\chi_{\Lambda_L}\Pi_b) = \int_{\Omega} \Pi_b(\underline{x}; \underline{x})d\underline{x}, \quad (2.4.7)$$

where the second inequality is a consequence of the \mathbb{Z}^2 -periodicity of $\Pi_b(\mathbf{x}; \mathbf{x})$, implied by (2.4.6).

Let X_j be the multiplication operator with x_j . Due to (2.4.2) we have that the commutators $[X_j, \Pi_b]$ have continuous integral kernels given by $(x_j - x'_j)\Pi_b(\mathbf{x}; \mathbf{x}')$ and which are exponentially localized near the diagonal. Due to the (2.4.6) we see that these commutators also commute with the magnetic translations. Again by (2.4.6), the integral kernel of $i\Pi_b [[X_1, \Pi_b], [X_2, \Pi_b]]$ is such that for all $\eta \in \mathbb{Z}^2$

$$\begin{aligned} & (i\Pi_b [[X_1, \Pi_b], [X_2, \Pi_b]]) (\mathbf{x}; \mathbf{x}') \\ &= e^{ib\phi(\eta,\mathbf{x})} (i\Pi_b [[X_1, \Pi_b], [X_2, \Pi_b]]) (\mathbf{x} - \eta; \mathbf{x}' - \eta)e^{-ib\phi(\eta,\mathbf{x}')}. \end{aligned}$$

The Chern character, according to Definition 2.1.3, is given by

$$C(\Pi_b) = 2\pi \int_{\Omega} (i\Pi_b [[X_1, \Pi_b], [X_2, \Pi_b]]) (\underline{x}; \underline{x})d\underline{x}. \quad (2.4.8)$$

We are now prepared to formulate our first main result, a gap labelling theorem for Bloch–Landau Hamiltonians.

Theorem 2.4.1. *Assume that H_b has an isolated spectral island σ_b which remains isolated and varies continuously in the Hausdorff distance as long as $b \in (b_1, b_2)$. Let Π_b be its corresponding spectral projection. Then:*

(i) *the map $(b_1, b_2) \ni b \mapsto \mathcal{I}(\Pi_b) \in \mathbb{R}$ is continuously differentiable and*

$$\frac{d\mathcal{I}(\Pi_b)}{db} = \frac{1}{2\pi}C(\Pi_b) \quad (2.4.9)$$

with $C(\Pi_b)$ as in (2.4.8);

(ii) *the Chern character is constant on (b_1, b_2) and*

$$C(\Pi_b) = c_1 \in \mathbb{Z};$$

Moreover, there exists a rational number $c_0 \in \mathbb{Q}$ such that

$$\mathcal{I}(\Pi_b) = c_0 + c_1 \frac{b}{2\pi}, \quad b \in (b_1, b_2). \quad (2.4.10)$$

As a by-product of the above gap labelling theorem, we can deduce information regarding the singularity of the magnetic perturbation. To formulate the statement more precisely, we will need the notion of a *localized Wannier-like basis*. In the present context, we say that the Fermi projection Π_b admits a localized Wannier-like basis if

$$\Pi_b(\mathbf{x}; \mathbf{x}') = \sum_{j=1}^M \sum_{\gamma \in \mathbb{Z}^2} \psi_{j,\gamma}(\mathbf{x}) \overline{\psi_{j,\gamma}(\mathbf{x}')}, \quad \psi_{j,\gamma}(\mathbf{x}) := e^{i\theta(\mathbf{x})} \tau_{b',\gamma} w_j(\mathbf{x}), \quad (2.4.11)$$

where $M \in \mathbb{N}$, $\theta: \mathbb{R}^2 \rightarrow \mathbb{R}$, $b' \in \mathbb{R}$, and the functions $w_j \in L^2(\mathbb{R}^2)$ are such that

$$|w_j(\underline{x} + \gamma)| \leq C e^{-\alpha\|\gamma\|} \quad (2.4.12)$$

for some $\alpha, C > 0$ uniform in $j \in \{1, \dots, M\}$ and $\underline{x} \in \Omega$. Notice that a localized Wannier-like basis is a particular type of generalized Wannier basis in the sense of Definition 1.3.6, where the role of the Delone set is played by the regular lattice \mathbb{Z}^2 . Moreover, a localized Wannier-like basis has a lot more structure than a generalized Wannier basis. Indeed, it has almost a ladder structure, in the sense that all the elements of the basis can be generated from a finite set of functions by first acting with a magnetic translation and then with a unitary operator. The reason behind this structure will be clarified in Chapter 5, compare with Corollary 5.4.3.

Corollary 2.4.2. *Under the same assumptions as in Theorem 2.4.1, the map $(b_1, b_2) \ni b \mapsto \Pi_b$ is everywhere continuous in the strong topology.*

Moreover, for $b \in (b_1, b_2)$, assume that either $c_1 \neq 0$ in (2.4.10), or $c_1 = 0$ and Π_b admits a localized Wannier-like basis. Then we have

$$\lim_{\epsilon \rightarrow 0} \|\Pi_{b+\epsilon} - \Pi_b\| = 1. \quad (2.4.13)$$

In particular, the above limit holds if $c_1 = 0$ and $b/(2\pi)$ is rational.

Remark 2.4.3. Corollary 2.4.2 highlights the singularity of the magnetic perturbation: the map $b \mapsto \Pi_b$ is everywhere continuous in the strong topology, but dramatically fails to be continuous in the norm topology.

While the case $c_1 \neq 0$ is a rather straightforward consequence of Theorem 2.4.1, the case $c_1 = 0$ is more involved. A less general situation of this case was already treated by Nenciu [86, Lemma 5.8]. He only considered $b = 0$ while σ_0 was a simple absolutely continuous band for which he assumed the existence of an orthonormal basis of exponentially localized Wannier functions. The strategy behind our proof is essentially the same as Nenciu's, but we generalize his argument in particular to any rational flux, by showing in Appendix 2.5.1 that also in this case one can construct an orthonormal basis of localized Wannier functions for the Fermi projection.

Motivated by magnetic perturbation theory (see Chapter 5, where (2.4.11) is shown to hold for certain perturbations around rational-flux Fermi projections), we conjecture that (2.4.13) and the existence of a localized Wannier-like basis as in (2.4.11) should also hold for all irrational fluxes when $c_1 = 0$.

Remark 2.4.4. The Chern character, also known as the real space Chern number, has been studied by Avron, Seiler and Simon in [9]. In that work the authors connect

the formula of the Chern character to the index of pair of projections, which is always an integer by construction. Hence, applying the results in [9] to our setting, one obtains that for values of b that do not close the gap of H_b , the Chern character is actually an integer. However, two comments are in order:

- the projection Π_b is not norm continuous with respect to b , see Corollary 2.4.2. Therefore, even though $C(\Pi_b)$ is an integer, in principle it could take different integer values for different values of b in the interval (b_1, b_2) ;
- the proof that the Chern character is an integer provided in [9] takes into account a more general setting (Landau Hamiltonian with disordered scalar potential) but relies on some results by Connes regarding non-commutative geometry. Indeed, quoting the authors word in [9]:

That such integrals can be evaluated explicitly, and have geometric significance is a result of Connes [28] and is a rather amazing fact.

Because of that we decided to exhibit a different, self consistent and in our opinion more evident proof of the Chern character integrality in the setting of the Bloch–Landau Hamiltonians.

Slowly varying magnetic perturbations

Here we discuss the generalization of the above Diophantine formula (2.4.10) to magnetic field perturbations that are slowly varying with respect to the lattice \mathbb{Z}^2 , in the sense of space adiabatic perturbation theory. Let $\mathcal{A}(\mathbf{x}) = (\mathcal{A}_1(x_1, x_2), \mathcal{A}_2(x_1, x_2))$ be a C^2 magnetic potential ⁴ and define $B := \partial_2 \mathcal{A}_1 - \partial_1 \mathcal{A}_2$. We assume that B is at least C^1 with bounded derivatives in the following way:

$$\sup_{\mathbf{x} \in \mathbb{R}^2} |\partial^\alpha B(\mathbf{x})| \leq C_\alpha, \quad \alpha \in \mathbb{N}^2, \quad |\alpha| \leq 1. \quad (2.4.14)$$

On top of that, we require that in the limit of large scales the magnetic field has a constant (positive) flux per unit area, that is

$$\langle B \rangle := \lim_{L \rightarrow \infty} \frac{1}{|\Lambda_L|} \int_{\Lambda_L} B(\mathbf{x}) d\mathbf{x} \geq 0. \quad (2.4.15)$$

Let $0 < \lambda \ll 1$ denote the slow variation parameter. Let us introduce $\mathcal{A}_\lambda(\mathbf{x}) := \mathcal{A}(\lambda \mathbf{x})$. Then \mathcal{A}_λ produces a weak and slowly varying magnetic field $B_\lambda(\mathbf{x}) := \lambda B(\lambda \mathbf{x})$. Let us consider the perturbed Hamiltonian of the form

$$H_{b,\lambda} := \frac{1}{2} (\mathbf{P} - b\mathbf{A} + \mathcal{A}_\lambda)^2 + V, \quad (2.4.16)$$

with b , \mathbf{A} and V as before. Up to a gauge transformation, we may assume that \mathcal{A}_λ is given in the transverse gauge:

$$\mathcal{A}_\lambda(\mathbf{x}) = \left(\int_0^1 s B_\lambda(s\mathbf{x}) ds \right) (-x_2, x_1). \quad (2.4.17)$$

⁴We incorporate in \mathcal{A} the factor $\frac{1}{c}$.

$H_{b,\lambda}$ remains essentially selfadjoint on $C_0^\infty(\mathbb{R}^2)$. As in the previous section, we assume that $H_{b,0}$ has an isolated spectral island $\sigma_{b,0}$. Since the perturbing magnetic field is of order λ , then for λ small enough the perturbation given by \mathcal{A}_λ does not close the gap between $\sigma_{b,0}$ and the rest of the spectrum [85, 87] (see also Appendix 2.5.2). Thus $H_{b,\lambda}$ still has a spectral island $\sigma_{b,\lambda}$ “close to” $\sigma_{b,0}$. Via a Riesz integral we can define $\Pi_{b,\lambda}$ to be the spectral projection onto the spectral island $\sigma_{b,\lambda}$.

The operator $H_{b,\lambda}$ is not necessarily covariant anymore (i.e., it need not commute with some magnetic translations) and we can no longer be sure that $\Pi_{b,\lambda}$ admits an integrated density of states in the sense of (2.4.7), namely the existence of the limit

$$\lim_{L \rightarrow \infty} p_{b,\lambda}^L, \quad \text{where} \quad p_{b,\lambda}^L := \frac{1}{|\Lambda_L|} \text{Tr}(\chi_L \Pi_{b,\lambda})$$

is not always guaranteed. Nevertheless, the \liminf and \limsup of $p_{b,\lambda}^L$ always exist because the sequence is bounded in L (see also (2.4.3)).

Now we are ready to state the second main result of this section.

Theorem 2.4.5. *Let $\Pi_{b,\lambda}$ be the spectral projection defined above. Denote by I_λ either $\limsup_{L \rightarrow \infty} p_{b,\lambda}^L$ or $\liminf_{L \rightarrow \infty} p_{b,\lambda}^L$. Then*

$$I_\lambda = \mathcal{I}(\Pi_{b,0}) + \lambda \frac{\langle B \rangle}{2\pi} C(\Pi_{b,0}) + \mathcal{O}(\lambda^2), \quad (2.4.18)$$

where $\langle B \rangle$ is defined in (2.4.15).

Remark 2.4.6. Theorem 2.4.5 says that even if the integrated density of states might not exist, the first order terms in λ of $\limsup_L p_{b,\lambda}^L$ and $\liminf_L p_{b,\lambda}^L$ are equal and proportional to the Chern character of the unperturbed projection, thus the possible failure in the existence of an IDS is only quadratic in λ .

2.4.2 Proof of Theorem 2.4.1 and Corollary 2.4.2

Proof of (i)

Let us fix some $b \in (b_1, b_2)$ and assume that $\epsilon \neq 0$ is such that $b + \epsilon \in (b_1, b_2)$. Proving (2.4.9) is equivalent to showing

$$\mathcal{I}(\Pi_{b+\epsilon}) = \mathcal{I}(\Pi_b) + \frac{\epsilon}{2\pi} C(\Pi_b) + o(\epsilon), \quad \epsilon \rightarrow 0. \quad (2.4.19)$$

It is well known in the literature [36, 87] that the constant magnetic field induces a singular perturbation. Fortunately, in order to compute $\mathcal{I}(\Pi_{b+\epsilon})$ we only need a good control on the diagonal value $\Pi_{b+\epsilon}(\mathbf{x}; \mathbf{x})$ of the integral kernel. The gauge covariant magnetic perturbation theory provides us with a convergent expansion in ϵ of exactly such objects.

First of all, we define the selfadjoint operator $\tilde{\Pi}^{(\epsilon)}$ given by the following integral kernel:

$$\tilde{\Pi}^{(\epsilon)}(\mathbf{x}; \mathbf{x}') = e^{i\epsilon\phi(\mathbf{x}, \mathbf{x}')} \Pi_b(\mathbf{x}; \mathbf{x}'). \quad (2.4.20)$$

Using the gauge covariant magnetic perturbation theory as in [87] (see also Appendix 2.5.2) one can show that there exist two constants $\alpha, K > 0$ such that

$$\left| \Pi_{b+\epsilon}(\mathbf{x}; \mathbf{x}') - \tilde{\Pi}^{(\epsilon)}(\mathbf{x}; \mathbf{x}') \right| \leq |\epsilon| K e^{-\alpha \|\mathbf{x} - \mathbf{x}'\|}. \quad (2.4.21)$$

In fact, as we have shown in Section 2.2.1, we could give an explicit formula for the difference in the left hand side in all orders of ϵ , but the expression is complicated and contains contributions coming from all spectral subspaces of H_b , not just from the one corresponding to Π_b . Using such an exact formula in order to show that the first order contribution in ϵ to $\mathcal{I}(\Pi_{b+\epsilon})$ is proportional to $C(\Pi_b)$ requires a careful preliminary massage to the Chern character formula, that in the end make the proof lengthy and not very transparent.

Instead, to prove (2.4.19) we will use a quite different strategy which only involves the integral kernel of Π_b , the knowledge that Π_b is a projection, and the a-priori zero-order estimate (2.4.21). This strategy consists of two steps:

Step 1. Using the fact that $\tilde{\Pi}^{(\epsilon)}$ is an “almost” projection, we will explicitly construct an auxiliary “true” projection $\mathcal{P}^{(\epsilon)}$ which, for $|\epsilon|$ small enough, is unitarily equivalent to $\Pi_{b+\epsilon}$. The estimate (2.4.21) implies that the unitary operator that intertwines the two projections has an integral kernel that is exponentially localized, see (2.4.26). Hence $\mathcal{P}^{(\epsilon)}$ has the same integrated density of states as $\Pi_{b+\epsilon}$ (see Lemma 2.4.7 below).

Step 2. We will study the asymptotic in ϵ of the integrated density of states of $\mathcal{P}^{(\epsilon)}$ and show that

$$\mathcal{I}(\mathcal{P}^{(\epsilon)}) = \mathcal{I}(\mathcal{P}^{(0)}) + \frac{\epsilon}{2\pi}C(\Pi_b) + o(\epsilon), \quad \epsilon \rightarrow 0. \quad (2.4.22)$$

Step 1

Define the operator

$$\Delta^{(\epsilon)} := (\tilde{\Pi}^{(\epsilon)})^2 - \tilde{\Pi}^{(\epsilon)}.$$

The operator $\Delta^{(\epsilon)}$ measures how far $\tilde{\Pi}^{(\epsilon)}$ is from being a projection. Using (2.4.2) and (2.4.5) one can prove (see (2.4.29) below and also Section 5.9.3) that if ϵ is small enough then

$$|\Delta^{(\epsilon)}(\mathbf{x}; \mathbf{x}')| \leq |\epsilon|K e^{-\alpha\|\mathbf{x}-\mathbf{x}'\|}. \quad (2.4.23)$$

Thus we can construct the following orthogonal projections (see also [87] for more details):

$$\mathcal{P}^{(\epsilon)} := \tilde{\Pi}^{(\epsilon)} + (\tilde{\Pi}^{(\epsilon)} - \frac{1}{2}\mathbf{1})\{(\mathbf{1} + 4\Delta^{(\epsilon)})^{-1/2} - \mathbf{1}\}. \quad (2.4.24)$$

Since the integral kernel of $\Delta^{(\epsilon)}$ is exponentially localized and of order ϵ , one can prove (see Lemma 5.8.5) that

$$\left| \{(\mathbf{1} + 4\Delta^{(\epsilon)})^{-1/2} - \mathbf{1} + 2\Delta^{(\epsilon)}\}(\mathbf{x}; \mathbf{x}') \right| \leq \epsilon^2 K e^{-\alpha\|\mathbf{x}-\mathbf{x}'\|} \quad (2.4.25)$$

This estimate, combined with definition (2.4.24) and with (2.4.21), yields the following pointwise estimate:

$$\left| (\Pi_{b+\epsilon} - \mathcal{P}^{(\epsilon)}) (\mathbf{x}; \mathbf{x}') \right| \leq K|\epsilon| e^{-\alpha\|\mathbf{x}-\mathbf{x}'\|}. \quad (2.4.26)$$

Due to (2.4.26) we have that $\|\Pi_{b+\epsilon} - \mathcal{P}^{(\epsilon)}\| \leq C|\epsilon| \leq 1/2$ when $|\epsilon|$ is sufficiently small, hence we can consider the Kato–Sz.–Nagy unitary operator U_ϵ [64] such that

$\Pi_{b+\epsilon} = U_\epsilon \mathcal{P}^{(\epsilon)} U_\epsilon^*$. From its explicit expression one can obtain the following estimate (cf. Lemma 5.8.5):

$$|(U_\epsilon - \mathbf{1})(\mathbf{x}; \mathbf{x}')| \leq C e^{-\alpha \|\mathbf{x} - \mathbf{x}'\|}, \quad (2.4.27)$$

which holds for some positive constants C and α , provided $|\epsilon|$ is small enough.

Now we prove that $\Pi_{b+\epsilon}$ and $\mathcal{P}^{(\epsilon)}$ have the same integrated density of states if $|\epsilon|$ is small enough. In order to do that, we use the following general lemma.

Lemma 2.4.7. *Let P_1 and P_2 be two orthogonal projections acting on $L^2(\mathbb{R}^2)$ such that their integral kernels satisfy (2.4.2). Assume that there exists a unitary operator U such that $P_1 = U P_2 U^*$ and whose integral kernel satisfies (2.4.27).*

Then we have

$$\lim_{L \rightarrow \infty} \frac{1}{|\Lambda_L|} |\mathrm{Tr}(\chi_L P_1) - \mathrm{Tr}(\chi_L P_2)| = 0.$$

In particular, if both P_1 and P_2 admit an integrated density of states like in (2.4.7), then $\mathcal{I}(P_1) = \mathcal{I}(P_2)$.

Proof. Reasoning as in (2.4.3) we observe that the operators $\chi_L P_1$, $\chi_L P_2$ and $\chi_L U P_2$ are trace class. Using the trace cyclicity we obtain the identity

$$\mathrm{Tr}(\chi_L P_1) - \mathrm{Tr}(\chi_L P_2) = \mathrm{Tr}([\chi_L, U] P_2 U^*).$$

Denoting by $W := U - \mathbf{1}$ we see from (2.4.27) that $W(\mathbf{x}; \mathbf{x}')$ is exponentially localized near the diagonal and

$$\mathrm{Tr}([\chi_L, U] P_2 U^*) = \mathrm{Tr}([\chi_L, W] P_2) + \mathrm{Tr}([\chi_L, W] P_2 W^*).$$

Both traces can be bounded by a double integral of the type

$$\int_{\mathbb{R}^2} d\mathbf{x}' \int_{\mathbb{R}^2} d\mathbf{x} e^{-\alpha \|\mathbf{x} - \mathbf{x}'\|} |\chi_L(\mathbf{x}) - \chi_L(\mathbf{x}')|.$$

In the above integral, the integrand is non-zero only if one variable belongs to Λ_L and the other one lies outside Λ_L . Due to the symmetry, it is enough to estimate

$$\int_{\Lambda_L} d\mathbf{x}' \int_{\mathbb{R}^2 \setminus \Lambda_L} d\mathbf{x} e^{-\alpha \|\mathbf{x} - \mathbf{x}'\|}.$$

For a fixed $\mathbf{x} \in \Lambda_L$ we have the inequality

$$e^{-\alpha \|\mathbf{x} - \mathbf{x}'\|} \leq e^{-\alpha \mathrm{dist}(\mathbf{x}, \partial \Lambda_L)/2} e^{-\alpha \|\mathbf{x} - \mathbf{x}'\|/2}, \quad \forall \mathbf{x}' \in \mathbb{R}^2 \setminus \Lambda_L.$$

By integrating with respect to \mathbf{x}' at fixed \mathbf{x} we can bound the above double integral by

$$\int_{\Lambda_L} d\mathbf{x} e^{-\alpha \mathrm{dist}(\mathbf{x}, \partial \Lambda_L)/2} \leq C L,$$

hence when dividing by $L^2 = |\Lambda_L|$ we obtain the claimed convergence to zero. \square

Using (2.4.6) one can prove by direct computation that the operator $\tilde{\Pi}^{(\epsilon)}$ commutes with the magnetic translations $\tau_{b+\epsilon, \eta}$. Since $\mathcal{P}^{(\epsilon)}$ is a function of $\tilde{\Pi}^{(\epsilon)}$, it also commutes with the same magnetic translations, thus $\tilde{\Pi}^{(\epsilon)}(\mathbf{x}; \mathbf{x})$ and $\mathcal{P}^{(\epsilon)}(\mathbf{x}; \mathbf{x})$ are periodic functions and the integrated densities of states $\mathcal{I}(\tilde{\Pi}^{(\epsilon)})$, $\mathcal{I}(\mathcal{P}^{(\epsilon)})$ exist. Due to (2.4.26) and (2.4.27) we can apply Lemma 2.4.7 to $\mathcal{P}^{(\epsilon)}$ and $\tilde{\Pi}^{(\epsilon)} = U_\epsilon \mathcal{P}^{(\epsilon)} U_\epsilon^*$ and conclude that

$$\mathcal{I}(\Pi_{b+\epsilon}) = \mathcal{I}(\mathcal{P}^{(\epsilon)}).$$

Step 2

We now prove (2.4.22). Let us begin by studying $\mathcal{P}^{(\epsilon)}$ in detail. Using the same method yielding (2.4.26) but taking into account also the term of order ϵ we obtain the estimate

$$\left| \mathcal{P}^{(\epsilon)}(\mathbf{x}; \mathbf{x}') - \left\{ \tilde{\Pi}^{(\epsilon)} - 2\tilde{\Pi}^{(\epsilon)}\Delta^{(\epsilon)} + \Delta^{(\epsilon)} \right\}(\mathbf{x}; \mathbf{x}') \right| \leq C\epsilon^2 e^{-\alpha\|\mathbf{x}-\mathbf{x}'\|}.$$

This leads to

$$\left| \mathcal{P}^{(\epsilon)}(\mathbf{x}; \mathbf{x}) - \mathcal{P}^{(0)}(\mathbf{x}; \mathbf{x}) - \left\{ -2\tilde{\Pi}^{(\epsilon)}\Delta^{(\epsilon)} + \Delta^{(\epsilon)} \right\}(\mathbf{x}; \mathbf{x}) \right| \leq C\epsilon^2, \quad (2.4.28)$$

where we used that $\tilde{\Pi}^{(\epsilon)}(\mathbf{x}; \mathbf{x}) = \Pi_b(\mathbf{x}; \mathbf{x}) = \mathcal{P}^{(0)}(\mathbf{x}; \mathbf{x})$, independent of ϵ .

Exploiting the composition rule for the Peierls phase (2.4.5), the fact that Π_b is a projection, and the exponential localization of the integral kernel of Π_b , we obtain

$$\begin{aligned} & \Delta^{(\epsilon)}(\mathbf{x}; \mathbf{x}') \\ &= \int_{\mathbb{R}^2} d\mathbf{y} \left(e^{i\epsilon\phi(\mathbf{x}, \mathbf{y})} \Pi_b(\mathbf{x}; \mathbf{y}) e^{i\epsilon\phi(\mathbf{y}, \mathbf{x}')} \Pi_b(\mathbf{y}; \mathbf{x}') - e^{i\epsilon\phi(\mathbf{x}, \mathbf{x}')} \Pi_b(\mathbf{x}; \mathbf{y}) \Pi_b(\mathbf{y}; \mathbf{x}') \right) \\ &= \frac{i}{2} e^{i\epsilon\phi(\mathbf{x}, \mathbf{x}')} \epsilon \int_{\mathbb{R}^2} d\mathbf{y} [(\mathbf{x} - \mathbf{y})_2 (\mathbf{y} - \mathbf{x}')_1 - (\mathbf{x} - \mathbf{y})_1 (\mathbf{y} - \mathbf{x}')_2] \Pi_b(\mathbf{x}; \mathbf{y}) \Pi_b(\mathbf{y}; \mathbf{x}') \\ & \quad + \mathcal{O}(\epsilon^2 e^{-\alpha\|\mathbf{x}-\mathbf{x}'\|}). \end{aligned} \quad (2.4.29)$$

Noticing that $\Delta^{(\epsilon)}(\mathbf{x}; \mathbf{x}) = 0 + \mathcal{O}(\epsilon^2)$ it follows that only $-2\tilde{\Pi}^{(\epsilon)}\Delta^{(\epsilon)}(\mathbf{x}; \mathbf{x})$ contributes to the first order expansion in ϵ of $\mathcal{P}^{(\epsilon)}(\mathbf{x}; \mathbf{x})$ in (2.4.28). More precisely

$$\begin{aligned} & -2 \left(\tilde{\Pi}^{(\epsilon)} \Delta^{(\epsilon)} \right) (\mathbf{x}; \mathbf{x}) \\ &= -2 \int_{\mathbb{R}^2} d\tilde{\mathbf{x}} e^{i\epsilon\phi(\mathbf{x}, \tilde{\mathbf{x}})} \Pi_b(\mathbf{x}; \tilde{\mathbf{x}}) \Delta^{(\epsilon)}(\tilde{\mathbf{x}}; \mathbf{x}) \\ &= i\epsilon \int_{\mathbb{R}^2} d\tilde{\mathbf{x}} \Pi_b(\mathbf{x}; \tilde{\mathbf{x}}) \int_{\mathbb{R}^2} d\mathbf{y} [(\tilde{\mathbf{x}} - \mathbf{y})_1 (\mathbf{y} - \mathbf{x})_2 - (\tilde{\mathbf{x}} - \mathbf{y})_2 (\mathbf{y} - \mathbf{x})_1] \Pi_b(\tilde{\mathbf{x}}; \mathbf{y}) \Pi_b(\mathbf{y}; \mathbf{x}) \\ & \quad + \mathcal{O}(\epsilon^2) \\ &= \epsilon (i\Pi_b [[X_1, \Pi_b], [X_2, \Pi_b]]) (\mathbf{x}; \mathbf{x}) + \mathcal{O}(\epsilon^2). \end{aligned}$$

This proves (2.4.22), see (2.4.8).

The continuity of $C(\Pi_b)$ as a function of $b \in (b_1, b_2)$ can be shown using the same method, i.e. by replacing $\Pi_{b+\epsilon}$ with $\tilde{\Pi}^{(\epsilon)}$ in the expression of $C(\Pi_{b+\epsilon})$ then using (2.4.21) and the composition rule (2.4.5) for the magnetic phases. In fact, one can prove infinite differentiability in this way.

Proof of (ii)

From Theorem 2.4.1 (i) we know that the derivative of the integrated density of states is a continuous function and it is proportional to the Chern character $C(\Pi_b)$ for every b restricted to compact intervals in (b_1, b_2) where the spectral island σ_b remains isolated from the rest of the spectrum.

The main observation, proved for the convenience of the reader in Appendix 2.5.1, is that the map

$$(b_1, b_2) \ni b \mapsto C(\Pi_b) \in \mathbb{R}$$

takes integer values when $b/(2\pi) \in \mathbb{Q}$. Since the map is at the same time uniformly continuous on any compact interval included in (b_1, b_2) , a straightforward argument shows that it must be constant and thus everywhere equal to an integer $c_1 \in \mathbb{Z}$.

In order to prove (2.4.10), let us fix some $b_0 \in (b_1, b_2)$ such that $b_0/(2\pi) = p/q \in \mathbb{Q}$. Then for every other b in this interval we have by (2.4.9)

$$\mathcal{I}(\Pi_b) = \mathcal{I}(\Pi_{b_0}) + c_1 \frac{b}{2\pi} - \frac{c_1 p}{q}.$$

In Appendix 2.5.1 we will prove that Π_{b_0} is a fibered operator. In the magnetic Bloch–Floquet representation, the fiber of Π_{b_0} at a fixed quasimomentum \mathbf{k} is a rank- M orthogonal projection. Also, σ_{b_0} is the union of M mini-bands (which might overlap). When we compute $\mathcal{I}(\Pi_{b_0})$ with the help of (2.5.5), the result is that $\mathcal{I}(\Pi_{b_0}) = M/q \in \mathbb{Q}$. Thus setting $c_0 := (M - c_1 p)/q$ concludes the proof.

2.4.3 Proof of Corollary 2.4.2

Continuity in strong topology is known since at least Kato [64], who used asymptotic perturbation theory. For the sake of the reader we present here a much shorter proof based on magnetic perturbation theory. By a standard density argument it is enough to show that

$$\lim_{\epsilon \rightarrow 0} \|(\Pi_{b+\epsilon} - \Pi_b)\psi\| = 0$$

for every ψ with compact support. This follows from (2.4.2), (2.4.20), (2.4.21), from the inequality

$$\left| e^{i\epsilon\phi(\mathbf{x}, \mathbf{x}')} - 1 \right| \leq |\epsilon| |\phi(\mathbf{x}, \mathbf{x}')| \leq |\epsilon| \|\mathbf{x} - \mathbf{x}'\| \|\mathbf{x}'\|/2$$

and the fact that $\|\mathbf{x}'\| |\psi(\mathbf{x}')|$ is in $L^2(\mathbb{R}^2)$.

Now let us continue with proving the discontinuity in norm topology. We start with a general fact: if P_1 and P_2 are orthogonal projections, then $\|P_1 - P_2\| \leq 1$ [64, Chap. I, Problem 6.33]. Hence in order to prove (2.4.13) it is enough to show that the \liminf cannot be less than one.

Let $c_1 \neq 0$. Assume that (2.4.13) is false. Then there would exist an $a \in [0, 1)$ and a sequence $\epsilon_n \neq 0$, depending on a , such that $\epsilon_n \rightarrow 0$ and $\lim_{n \rightarrow \infty} \|\Pi_{b+\epsilon_n} - \Pi_b\| = a$. This implies the existence of some n_0 such that for every $n \geq n_0$ we have

$$\|\Pi_{b+\epsilon_n} - \Pi_b\| \leq \frac{(1+a)}{2} < 1.$$

Then $\Pi_{b+\epsilon_n}$ and Π_b would be intertwined by a Kato–Sz.-Nagy unitary. Let us now prove that the Kato–Sz.-Nagy unitary satisfies (2.4.27). Fix $n > n_0$ and define the operator $D_n := \Pi_{b+\epsilon_n} - \Pi_b$. Since the kernel of both operators is exponentially localized, see (2.4.2), one can find two constants α and C that does not depend on n , such that

$$|D_n(\mathbf{x}; \mathbf{x}')| \leq C e^{-\alpha\|\mathbf{x}-\mathbf{x}'\|}. \quad (2.4.30)$$

Then, for all $0 \leq \delta < \delta_0 < \alpha$, it holds

$$\left| D_n(\mathbf{x}; \mathbf{x}') e^{\delta\|\mathbf{x}-\mathbf{x}'\|} - D_n(\mathbf{x}; \mathbf{x}') \right| \leq C \delta e^{-\frac{\alpha}{2}\|\mathbf{x}-\mathbf{x}'\|}, \quad (2.4.31)$$

which is a simple consequence of $|e^{\|\mathbf{x}\|} - 1| \leq \|\mathbf{x}\|e^{\|\mathbf{x}\|}$. Hence, choosing δ small enough, using the triangle inequality and (2.4.31) together with a Schur–Holmgren estimate, we obtain

$$\sup_{\mathbf{x}_0 \in \mathbb{R}^2} \left\| e^{\pm\delta\|\cdot - \mathbf{x}_0\|} D_n e^{\mp\delta\|\cdot - \mathbf{x}_0\|} \right\| < 1. \quad (2.4.32)$$

From the explicit formula of the Kato–Sz.-Nagy unitary U_n that intertwines $\Pi_{b+\epsilon_n}$ and Π_b , one has that

$$U_n - \mathbf{1} = \left((\mathbf{1} - D_n^2)^{-\frac{1}{2}} - \mathbf{1} \right) (\mathbf{1} + 2\Pi_{b+\epsilon_n}\Pi_b - \Pi_b - \Pi_{b+\epsilon_n}) + 2\Pi_{b+\epsilon_n}\Pi_b - \Pi_b - \Pi_{b+\epsilon_n}.$$

Since the projections $\Pi_{b+\epsilon_n}$ and Π_b have an exponentially localized integral kernel, see (2.4.2), we only have to prove that the operator $\left((\mathbf{1} - D_n^2)^{-\frac{1}{2}} - \mathbf{1} \right)$ has an integral kernel that satisfies (2.4.27). Therefore, consider

$$\begin{aligned} \left((\mathbf{1} - D_n^2)^{-\frac{1}{2}} - \mathbf{1} \right) &= D_n \left(\sum_{k=0}^{\infty} \frac{(2k+1)!!}{(k+1)!2^{(k+1)}} (D_n)^{2k} \right) D_n \\ &=: D_n \left(\sum_{k=0}^{\infty} t_k (D_n)^{2k} \right) D_n. \end{aligned}$$

From the estimate (2.4.32) we get that

$$\sup_{\mathbf{x}_0 \in \mathbb{R}^2} \left\| e^{-\delta\|\cdot - \mathbf{x}_0\|} \left(\sum_{k=0}^{\infty} t_k (D_n)^{2k} \right) e^{\delta\|\cdot - \mathbf{x}_0\|} \right\| \leq C.$$

Moreover, from the estimate $\left| e^{-\delta\|\mathbf{x} - \mathbf{x}_0\|} D_n(\mathbf{x}; \mathbf{x}') e^{\delta\|\mathbf{x}' - \mathbf{x}_0\|} \right| \leq C e^{-\frac{\delta}{2}\|\mathbf{x} - \mathbf{x}'\|}$ and the Cauchy-Schwarz inequality, one deduces that

$$\sup_{\mathbf{x}_0 \in \mathbb{R}^2} \left\| e^{-\delta\|\cdot - \mathbf{x}_0\|} D_n e^{\delta\|\cdot - \mathbf{x}_0\|} \right\|_{\mathcal{B}(L^2, L^\infty)} \leq C.$$

The previous two estimates imply that

$$\sup_{\mathbf{x}_0 \in \mathbb{R}^2} \left\| e^{-\delta\|\cdot - \mathbf{x}_0\|} D_n \left(\sum_{k=0}^{\infty} t_k (D_n)^{2k-1} \right) D_n e^{\delta\|\cdot - \mathbf{x}_0\|} \right\|_{\mathcal{B}(L^2, L^\infty)} \leq C,$$

hence $e^{-\delta\|\cdot - \mathbf{x}_0\|} \left(\sum_{k=0}^{\infty} t_k (D_n)^{2k} \right) D_n e^{\delta\|\cdot - \mathbf{x}_0\|}$ is a Carleman operator and in particular has an integral kernel. Furthermore, notice that $\Pi_{b+\epsilon}$ and Π_b map the Hilbert space into the space of continuous functions (see Section A.1.1), hence also the operator $e^{-\delta\|\cdot - \mathbf{x}_0\|} \left(\sum_{k=0}^{\infty} t_k (D_n)^{2k} \right) D_n e^{\delta\|\cdot - \mathbf{x}_0\|}$ shares the same property. Therefore, by mimicking the strategy in [37] and extensively revised in Section A.1, we can show that

$$\begin{aligned} &\sup_{\mathbf{x}_0 \in \mathbb{R}^2} \left\| e^{\delta\|\cdot - \mathbf{x}_0\|} \left(\sum_{k=0}^{\infty} t_k (D_n)^{2k+1} \right) (\mathbf{x}_0; \cdot) \right\|_{L^2(\mathbb{R}^2)} \\ &= \sup_{\mathbf{x}_0 \in \mathbb{R}^2} \left\| e^{\delta\|\cdot - \mathbf{x}_0\|} \left(\sum_{k=0}^{\infty} t_k (D_n)^{2k+1} \right) (\cdot; \mathbf{x}_0) \right\|_{L^2(\mathbb{R}^2)} \leq C. \end{aligned} \quad (2.4.33)$$

Using this, together with (2.4.30), the Cauchy-Schwarz and the triangle inequality, we eventually obtain that

$$\begin{aligned}
& \sup_{\mathbf{x}, \mathbf{x}'} e^{\delta \|\mathbf{x} - \mathbf{x}'\|} \left| \left((\mathbf{1} - D_n^2)^{-\frac{1}{2}} - \mathbf{1} \right) (\mathbf{x}; \mathbf{x}') \right| \\
& \leq \sup_{\mathbf{x}, \mathbf{x}'} \int_{\mathbb{R}^2} d\tilde{\mathbf{x}} e^{\delta \|\mathbf{x} - \tilde{\mathbf{x}}\|} |D_n(\mathbf{x}; \tilde{\mathbf{x}})| e^{\delta \|\tilde{\mathbf{x}} - \mathbf{x}'\|} \left| \left(\sum_{k=0}^{\infty} t_k (D_n)^{2k+1} \right) (\tilde{\mathbf{x}}; \mathbf{x}') \right| \\
& \leq \sup_{\mathbf{x} \in \mathbb{R}^2} \left\| e^{\delta \|\cdot - \mathbf{x}\|} |D_n(\mathbf{x}; \cdot)| \right\|_{L^2(\mathbb{R}^2)} \sup_{\mathbf{x}' \in \mathbb{R}^2} \left\| e^{\delta \|\cdot - \mathbf{x}'\|} \left| \left(\sum_{k=0}^{\infty} t_k (D_n)^{2k+1} \right) (\cdot; \mathbf{x}') \right| \right\|_{L^2(\mathbb{R}^2)} \\
& \leq C.
\end{aligned}$$

Thus the unitary U_n obeys the conditions of Lemma 2.4.7, hence $\mathcal{I}(\Pi_{b+\epsilon_n}) = \mathcal{I}(\Pi_b)$ if n is large enough, which contradicts that $c_1 \neq 0$.

Now let $c_1 = 0$, and assume (2.4.11). Let us define the unit vector

$$\Psi_{\epsilon, \eta}(\mathbf{x}) := e^{i\epsilon\phi(\mathbf{x}, \eta)} \psi_{1, \eta}(\mathbf{x}), \quad \eta \in \mathbb{Z}^2.$$

Using (2.4.20), (2.4.21), and the exponential decay (2.4.12) of w_1 we obtain the existence of $C > 0$ such that for all η

$$\langle \Psi_{\epsilon, \eta}, \Pi_{b+\epsilon} \Psi_{\epsilon, \eta} \rangle \geq 1 - C |\epsilon|.$$

Also

$$\|\Pi_{b+\epsilon} - \Pi_b\| \geq \langle \Psi_{\epsilon, \eta}, (\Pi_{b+\epsilon} - \Pi_b) \Psi_{\epsilon, \eta} \rangle \geq 1 - C |\epsilon| - \sum_{j=1}^M \sum_{\gamma \in \mathbb{Z}^2} |\langle \Psi_{\epsilon, \eta}, \psi_{j, \gamma} \rangle|^2.$$

Since the left hand side is independent of η we have the inequality

$$\|\Pi_{b+\epsilon} - \Pi_b\| \geq 1 - C |\epsilon| - \inf_{\eta \in \mathbb{Z}^2} \sum_{j=1}^M \sum_{\gamma \in \mathbb{Z}^2} |\langle \Psi_{\epsilon, \eta}, \psi_{j, \gamma} \rangle|^2. \quad (2.4.34)$$

We will now show that

$$\lim_{|\eta| \rightarrow \infty} \sum_{j=1}^M \sum_{\gamma \in \mathbb{Z}^2} |\langle \Psi_{\epsilon, \eta}, \psi_{j, \gamma} \rangle|^2 = 0,$$

which inserted in (2.4.34) would finish the proof. By changing γ into $\eta + \gamma$ we will investigate

$$\sum_{\gamma \in \mathbb{Z}^2} |\langle \Psi_{\epsilon, \eta}, \psi_{j, \eta + \gamma} \rangle|^2.$$

Due to the exponential localization of the w_j 's and using the triangle inequality one can prove the existence of two constants $\alpha, C > 0$ such that

$$|\langle \Psi_{\epsilon, \eta}, \psi_{j, \eta + \gamma} \rangle| \leq C e^{-\alpha \|\gamma\|}, \quad \forall \eta \in \mathbb{Z}^2.$$

Thus the proof would be over if we can prove that for fixed γ we have

$$\lim_{|\eta| \rightarrow \infty} \langle \Psi_{\epsilon, \eta}, \psi_{j, \eta + \gamma} \rangle = 0.$$

Let us compute

$$\begin{aligned} \langle \Psi_{\epsilon, \eta}, \psi_{j, \gamma + \eta} \rangle &= \langle e^{i\epsilon\phi(\cdot, \eta)} e^{i\theta(\cdot)} \tau_{b', \eta} w_1, e^{i\theta(\cdot)} \tau_{b', \gamma + \eta} w_j \rangle \\ &= \langle e^{i\epsilon\phi(\cdot, \eta)} \tau_{b', \eta} w_1, e^{i\theta(\cdot)} \tau_{b', \eta} \tau_{b', \gamma} w_j \rangle, \end{aligned}$$

where we used the fact that magnetic translations form a projective representation of \mathbb{Z}^2 . An easy computation, exploiting $\phi(\eta, \eta) = 0$, shows that multiplication by the phase factor $e^{i\epsilon\phi(\cdot, \eta)}$ commutes with the magnetic translation $\tau_{b', \eta}$. Up to a factor of modulus one, the above scalar product is then proportional to the integral

$$\int_{\mathbb{R}^2} e^{-i\epsilon\phi(\mathbf{x}, \eta)} \overline{w_1(\mathbf{x})} e^{i\theta(\mathbf{x}, \eta)} w_j(\mathbf{x} - \eta) d\mathbf{x}$$

where $[\mathbf{x}] \in \mathbb{Z}^2$ denotes the ‘‘integer part’’ in the decomposition $\mathbf{x} = \underline{x} + [\mathbf{x}]$ with $\underline{x} \in \Omega$. The above integral is proportional to the Fourier transform of the L^1 function

$$\overline{w_1(\mathbf{x})} e^{i\theta(\mathbf{x}, \eta)} w_j(\mathbf{x} - \eta),$$

evaluated at the point $\xi = \frac{\epsilon}{2}(-\eta_2, \eta_1)$. Since η is fixed and $\epsilon \neq 0$, the Riemann-Lebesgue lemma implies that the integral goes to zero when $|\eta| \rightarrow \infty$. The proof of Corollary 2.4.2 is over.

2.4.4 Proof of Theorem 2.4.5

The strategy of the proof resembles that of Theorem 2.4.1. In this section we denote by $\Pi_\lambda \equiv \Pi_{b, \lambda}$ the Fermi projection on the isolated spectral island $\sigma_{b, \lambda}$ of $H_{b, \lambda}$. We start by showing the existence of an auxiliary projection $\mathfrak{P}^{(\lambda)}$, unitarily equivalent to Π_λ , which can be used to explicitly compute the first order expansion in λ of I_λ in Theorem 2.4.5.

Let us introduce the phase factor given by

$$\phi_\lambda(\mathbf{x}, \mathbf{x}') := \int_{\mathbf{x}}^{\mathbf{x}'} \mathcal{A}_\lambda \equiv \int_0^1 \mathcal{A}_\lambda(\mathbf{x}' + s(\mathbf{x} - \mathbf{x}')) \cdot (\mathbf{x} - \mathbf{x}') ds. \quad (2.4.35)$$

Note that when \mathcal{A}_λ (see (2.4.16)) comes from a constant magnetic field, we obtain the usual Peierls phase (2.4.4).

Using results from magnetic perturbation theory [87] (see also Appendix 2.5.2) we have

$$|\Pi_\lambda(\mathbf{x}; \mathbf{x}') - e^{i\phi_\lambda(\mathbf{x}, \mathbf{x}')} \Pi_0(\mathbf{x}; \mathbf{x}')| \leq C\lambda e^{-\beta\|\mathbf{x} - \mathbf{x}'\|}. \quad (2.4.36)$$

As before, we define the operator $\tilde{\Pi}_\lambda$ through its integral kernel:

$$\tilde{\Pi}_\lambda(\mathbf{x}; \mathbf{x}') := e^{i\phi_\lambda(\mathbf{x}, \mathbf{x}')} \Pi_0(\mathbf{x}; \mathbf{x}').$$

We also define the auxiliary projection $\mathfrak{P}^{(\lambda)}$ (the analogue of $\mathcal{P}^{(\epsilon)}$ from the previous section) as

$$\mathfrak{P}^{(\lambda)} := \tilde{\Pi}_\lambda + (\tilde{\Pi}_\lambda - \frac{1}{2}\mathbf{1}) \{(\mathbf{1} + 4\Delta^{(\lambda)})^{-1/2} - \mathbf{1}\}, \quad \Delta^{(\lambda)} := \tilde{\Pi}_\lambda^2 - \tilde{\Pi}_\lambda, \quad (2.4.37)$$

such that

$$\left| (\Pi_\lambda - \mathfrak{P}^{(\lambda)})(\mathbf{x}; \mathbf{x}') \right| \leq C\lambda e^{-\alpha\|\mathbf{x} - \mathbf{x}'\|}. \quad (2.4.38)$$

From this, one can prove, see Section 5.8.1, that if λ is small enough, then one can construct the Kato–Sz.-Nagy unitary $U^{(\lambda)}$ such that $\Pi_\lambda = U^{(\lambda)}\mathfrak{P}^{(\lambda)}U^{(\lambda)*}$ and moreover

$$\left| (U^{(\lambda)} - \mathbf{1})(\mathbf{x}; \mathbf{x}') \right| \leq C e^{-\alpha \|\mathbf{x} - \mathbf{x}'\|}. \quad (2.4.39)$$

Now we are ready to prove equation (2.4.18). We only show the proof for the lim sup case since the lim inf case is completely analogous.

The operator $\chi_L \mathfrak{P}^{(\lambda)}$ is trace class (cf. (2.4.3)) and we have the trivial identity

$$\frac{1}{|\Lambda_L|} \text{Tr}(\chi_L \Pi_\lambda) = \frac{1}{|\Lambda_L|} \left(\text{Tr}(\chi_L \Pi_\lambda) - \text{Tr}(\chi_L \mathfrak{P}^{(\lambda)}) \right) + \frac{1}{|\Lambda_L|} \text{Tr}(\chi_L \mathfrak{P}^{(\lambda)}).$$

Thanks to Lemma 2.4.7, the first term on the right hand side of the above identity converges to zero as $L \rightarrow \infty$, hence taking the lim sup of both sides yields

$$I_\lambda = \limsup_{L \rightarrow \infty} \frac{1}{|\Lambda_L|} \text{Tr}(\chi_L \mathfrak{P}^{(\lambda)}). \quad (2.4.40)$$

What we have to prove now is that

$$\limsup_{L \rightarrow \infty} \frac{1}{|\Lambda_L|} \text{Tr}(\chi_L \mathfrak{P}^{(\lambda)}) = \mathcal{I}(\Pi_0) + \lambda \frac{\langle B \rangle}{2\pi} C(\Pi_0) + \mathcal{O}(\lambda^2). \quad (2.4.41)$$

As we have done in the case of a constant magnetic field, we need to study the expansion in λ of the trace on the left hand side of (2.4.41) using (2.4.37), and control the behaviour at large L . We separately analyse each term of (2.4.37).

Denote by $f_\lambda(\mathbf{x}, \mathbf{y}, \mathbf{x}')$ the magnetic flux generated by the slowly varying magnetic perturbation through the triangle $\langle \mathbf{x}, \mathbf{y}, \mathbf{x}' \rangle$ with corners situated at \mathbf{x} , \mathbf{y} and \mathbf{x}' :

$$f_\lambda(\mathbf{x}, \mathbf{y}, \mathbf{x}') = \phi_\lambda(\mathbf{x}, \mathbf{y}) + \phi_\lambda(\mathbf{x}, \mathbf{x}') - \phi_\lambda(\mathbf{y}, \mathbf{x}') = \int_{\langle \mathbf{x}, \mathbf{y}, \mathbf{x}' \rangle} \lambda B(\lambda \tilde{\mathbf{x}}) d\tilde{\mathbf{x}}. \quad (2.4.42)$$

Since B has uniformly bounded derivatives (see (2.4.14)), we obtain

$$|f_\lambda(\mathbf{x}, \mathbf{y}, \mathbf{x}')| \leq \lambda C_B \|\mathbf{x} - \mathbf{y}\| \|\mathbf{y} - \mathbf{x}'\| \quad (2.4.43)$$

with C_B a positive constant that only depends on the magnetic field B . Using equations (2.4.38), (2.4.42), and the fact that \mathfrak{P}_λ is a projection we obtain

$$\begin{aligned} \Delta^{(\lambda)}(\mathbf{x}; \mathbf{x}') &= \int_{\mathbb{R}^2} e^{i\phi_\lambda(\mathbf{x}, \mathbf{y})} \Pi_\lambda(\mathbf{x}; \mathbf{y}) e^{i\phi_\lambda(\mathbf{y}, \mathbf{x}')} \Pi_\lambda(\mathbf{y}; \mathbf{x}') d\mathbf{y} - e^{i\phi_\lambda(\mathbf{x}, \mathbf{x}')} \Pi_\lambda(\mathbf{x}; \mathbf{x}') \\ &= e^{i\phi_\lambda(\mathbf{x}, \mathbf{x}')} \int_{\mathbb{R}^2} e^{if_\lambda(\mathbf{x}, \mathbf{y}, \mathbf{x}')} \Pi_\lambda(\mathbf{x}; \mathbf{y}) \Pi_\lambda(\mathbf{y}; \mathbf{x}') d\mathbf{y} - e^{i\phi_\lambda(\mathbf{x}, \mathbf{x}')} \Pi_\lambda(\mathbf{x}; \mathbf{x}') \\ &= e^{i\phi_\lambda(\mathbf{x}, \mathbf{x}')} i \int_{\mathbb{R}^2} f_\lambda(\mathbf{x}, \mathbf{y}, \mathbf{x}') \Pi_\lambda(\mathbf{x}; \mathbf{y}) \Pi_\lambda(\mathbf{y}; \mathbf{x}') d\mathbf{y} + \mathcal{O}(\lambda^2 e^{-\alpha \|\mathbf{x} - \mathbf{x}'\|}). \end{aligned}$$

Given two vectors \mathbf{x} and \mathbf{y} we denote by $\{\mathbf{x} \wedge \mathbf{y}\} := x_1 y_2 - x_2 y_1$. From (2.4.42) we have

$$f_\lambda(\mathbf{x}, \mathbf{y}, \mathbf{x}') = \frac{\lambda}{2} B(\lambda \mathbf{x}') \{(\mathbf{x} - \mathbf{y}) \wedge (\mathbf{y} - \mathbf{x}')\} + \int_{\langle \mathbf{x}, \mathbf{y}, \mathbf{x}' \rangle} \lambda (B(\lambda \tilde{\mathbf{x}}) - B(\lambda \mathbf{x}')) d\tilde{\mathbf{x}}. \quad (2.4.44)$$

From (2.4.14) we deduce that B is a Lipschitz function:

$$|B(\mathbf{x}) - B(\mathbf{x}')| \leq K_B \|\mathbf{x} - \mathbf{x}'\|, \quad \forall \mathbf{x}, \mathbf{x}' \in \mathbb{R}^2. \quad (2.4.45)$$

Using the above estimate, the fact that the diameter of a triangle is less than the sum of the lengths of any two of its sides, and knowing that the area of the triangle is less than the product of the same two side-lengths, we get

$$\begin{aligned} & \left| \int_{\langle \mathbf{x}, \mathbf{y}, \mathbf{x}' \rangle} \lambda (B(\lambda \tilde{\mathbf{x}}) - B(\lambda \mathbf{x}')) d\tilde{\mathbf{x}} \right| \\ & \leq \lambda^2 K_B \left(\|\mathbf{x} - \mathbf{y}\|^2 \|\mathbf{y} - \mathbf{x}'\| + \|\mathbf{x} - \mathbf{y}\| \|\mathbf{y} - \mathbf{x}'\|^2 \right). \end{aligned} \quad (2.4.46)$$

Therefore, exploiting (2.4.44), (2.4.46) and the exponential localization of the integral kernel of Π_λ , we obtain

$$\begin{aligned} & \Delta^{(\lambda)}(\mathbf{x}; \mathbf{x}') \\ & = i\lambda \int_{\mathbb{R}^2} d\mathbf{y} B(\lambda \mathbf{x}') \frac{1}{2} \{(\mathbf{x} - \mathbf{y}) \wedge (\mathbf{y} - \mathbf{x}')\} \Pi_\lambda(\mathbf{x}; \mathbf{y}) \Pi_\lambda(\mathbf{y}; \mathbf{x}') + \mathcal{O}(\lambda^2 e^{-\alpha \|\mathbf{x} - \mathbf{x}'\|}). \end{aligned}$$

Putting $\mathbf{x} = \mathbf{x}'$ in the above equation we see that $\Delta^{(\lambda)}(\mathbf{x}; \mathbf{x}) = \mathcal{O}(\lambda^2)$ thus $\Delta^{(\lambda)}$ gives no contributions of order zero or λ to $|\Lambda_L|^{-1} \text{Tr} \left(\chi_L \mathfrak{P}^{(\lambda)} \right)$, uniformly in $L \geq 1$ (cf. the argument below (2.4.28)).

For the next term in the expansion (2.4.37) we have

$$\begin{aligned} & -2 \left(\mathfrak{P}^{(\lambda)} \Delta^{(\lambda)} \right) (\mathbf{x}; \mathbf{x}) \\ & = i\lambda B(\lambda \mathbf{x}) \int_{\mathbb{R}^2} d\tilde{\mathbf{x}} \Pi_0(\mathbf{x}; \tilde{\mathbf{x}}) \\ & \quad \cdot \int_{\mathbb{R}^2} d\mathbf{y} [(\tilde{\mathbf{x}} - \mathbf{y})_1 (\mathbf{y} - \mathbf{x})_2 - (\tilde{\mathbf{x}} - \mathbf{y})_2 (\mathbf{y} - \mathbf{x})_1] \Pi_0(\tilde{\mathbf{x}}; \mathbf{y}) \Pi_0(\mathbf{y}; \mathbf{x}) \\ & \quad + \mathcal{O}(\lambda^2) \\ & = \lambda B(\lambda \mathbf{x}) (i\Pi_0 [[X_1, \Pi_0], [X_2, \Pi_0]]) (\mathbf{x}; \mathbf{x}) + \mathcal{O}(\lambda^2). \end{aligned}$$

Thus we need to understand the behaviour of

$$\limsup_{L \rightarrow \infty} \frac{1}{|\Lambda_L|} \int_{\Lambda_L} B(\lambda \mathbf{x}) (i\Pi_0 [[X_1, \Pi_0], [X_2, \Pi_0]]) (\mathbf{x}; \mathbf{x}) d\mathbf{x}.$$

Because the integrand is uniformly bounded, it is enough to consider integer values for L , and in order to simplify the notation we assume that $L = 2L' + 1$ with $L' \in \mathbb{N}$. In this case we have

$$\Lambda_L = \{\mathbf{x} = \underline{x} + \gamma, \quad \underline{x} \in \Omega, \quad |\gamma_j| \leq L'\}.$$

Let us denote by $\mathfrak{C}(\mathbf{x}) := (i\Pi_0 [[X_1, \Pi_0], [X_2, \Pi_0]]) (\mathbf{x}; \mathbf{x})$. We have that $\mathfrak{C}(\underline{x} + \gamma) = \mathfrak{C}(\underline{x})$ for every $\underline{x} \in \Omega$ and $\gamma \in \mathbb{Z}^2$. Moreover

$$\int_{\Lambda_L} B(\lambda \mathbf{x}) \mathfrak{C}(\mathbf{x}) d\mathbf{x} = \sum_{|\gamma_j| \leq L'} \int_{\Omega} B(\lambda \underline{x} + \lambda \gamma) \mathfrak{C}(\underline{x}) d\underline{x}$$

$$\begin{aligned}
&= \sum_{|\gamma_j| \leq L'} \int_{\Omega} B(\lambda\gamma) \mathfrak{C}(\underline{x}) d\underline{x} \\
&+ \sum_{|\gamma_j| \leq L'} \int_{\Omega} (B(\lambda\underline{x} + \lambda\gamma) - B(\lambda\gamma)) \mathfrak{C}(\underline{x}) d\underline{x} \\
&= \frac{C(\Pi_0)}{2\pi} \sum_{|\gamma_j| \leq L'} B(\lambda\gamma) + \lambda \mathcal{O}(L^2)
\end{aligned}$$

by (2.4.45). Therefore, in view of (2.4.15), in order to complete the proof it suffices to show that

$$\limsup_{L \rightarrow \infty} \left| \frac{1}{|\Lambda_L|} \sum_{|\gamma_j| \leq L'} B(\lambda\gamma) - \frac{1}{|\Lambda_{\lambda L}|} \int_{\Lambda_{\lambda L}} B(\mathbf{x}) d\mathbf{x} \right| = \mathcal{O}(\lambda). \quad (2.4.47)$$

This is a consequence of the formula $|\Lambda_L| = \lambda^{-2} |\Lambda_{\lambda L}|$ and of (2.4.45). Indeed a computation similar to the above yields

$$\lambda^2 B(\lambda\gamma) = \int_{|x_j - \lambda\gamma_j| \leq \lambda/2} B(\mathbf{x}) d\mathbf{x} + \mathcal{O}(\lambda^3),$$

which gives (2.4.47) upon summing over $\gamma \in \Lambda_L \cap \mathbb{Z}^2$. In turn, using (2.4.15), the estimate (2.4.47) can be rewritten as

$$\limsup_{L \rightarrow \infty} \frac{1}{|\Lambda_L|} \sum_{|\gamma_j| \leq L'} B(\lambda\gamma) = \langle B \rangle + \mathcal{O}(\lambda).$$

This ends the proof of Theorem 2.4.5.

2.5 Appendix

2.5.1 Bloch–Floquet(–Zak) transform and the Chern number

In this appendix we discuss the magnetic Bloch–Floquet transform and the Chern character. The discussion is adapted to the special class of integral operators we work with.

Let $b_0 = 2\pi p/q$ for some p, q co-prime integer numbers and define the (modified) magnetic translation of vector $\eta \in \mathbb{Z}^2$, $\widehat{\tau}_{b_0, \eta}$, to be the following unitary operator:

$$(\widehat{\tau}_{b_0, \eta} f)(\mathbf{x}) := e^{ib_0 \eta_1 \eta_2 / 2} e^{ib_0 \phi(\mathbf{x}, \eta)} f(\mathbf{x} - \eta), \quad \forall f \in L^2(\mathbb{R}^2). \quad (2.5.1)$$

By direct computation one can prove that the set $\{\widehat{\tau}_{b_0, \gamma}\}_{\gamma \in \mathbb{Z}^2}$ forms a unitary projective representation of the group \mathbb{Z}^2 , that is

$$\widehat{\tau}_{b_0, \gamma} \widehat{\tau}_{b_0, \xi} = e^{-ib_0 \gamma_2 \xi_1} \widehat{\tau}_{b_0, \gamma + \xi}, \quad \forall \gamma, \xi \in \mathbb{Z}^2.$$

Considering the enlarged lattice

$$\mathbb{Z}_{(q)}^2 := \left\{ \eta \in \mathbb{Z}^2 \mid \eta = (\gamma_1, q\gamma_2), \gamma \in \mathbb{Z}^2 \right\},$$

we have that $\{\widehat{\tau}_{b_0, \eta}\}_{\eta \in \mathbb{Z}_{(q)}^2}$ is a true unitary representation of $\mathbb{Z}_{(q)}^2$, that is

$$\widehat{\tau}_{b_0, \eta} \widehat{\tau}_{b_0, \rho} = \widehat{\tau}_{b_0, \eta + \rho}, \quad \forall \eta, \rho \in \mathbb{Z}_{(q)}^2.$$

Let us denote by $\mathbb{Z}_{(q)}^{2*}$ the dual lattice of $\mathbb{Z}_{(q)}^2$ and by $\mathbb{B}_{(q)}$ and $\Omega_{(q)}$ the unit cells of $\mathbb{Z}_{(q)}^{2*}$ and $\mathbb{Z}_{(q)}^2$ respectively, i.e.

$$\mathbb{B}_{(q)} := (-\pi, \pi] \times (-\pi/q, \pi/q], \quad \Omega_{(q)} := (-1/2, 1/2] \times (-q/2, q/2].$$

$\mathbb{B}_{(q)}$ is usually called the (magnetic) Brillouin zone. We introduce the Bloch–Floquet unitary (denoted by \mathcal{U}_{BF}) as the operator which maps $L^2(\mathbb{R}^2)$ onto $\int_{\mathbb{B}_{(q)}}^{\oplus} L^2(\Omega_{(q)}) d\mathbf{k}$ and acts on $f \in C_0^\infty(\mathbb{R}^2)$ as

$$(\mathcal{U}_{BF} f)(\mathbf{k}, \underline{y}) := \frac{1}{|\mathbb{B}_{(q)}|^{1/2}} \sum_{\gamma \in \mathbb{Z}_{(q)}^2} e^{-i\mathbf{k} \cdot \gamma} (\widehat{\tau}_{b_0, -\gamma} f)(\underline{y}), \quad \mathbf{k} \in \mathbb{B}_{(q)}, \quad \underline{y} \in \Omega_{(q)}.$$

Its adjoint acts in the following way:

$$(\mathcal{U}_{BF}^* \psi)(\underline{y} + \eta) = \frac{1}{|\mathbb{B}_{(q)}|^{1/2}} \int_{\mathbb{B}_{(q)}} e^{i\mathbf{k} \cdot \eta} e^{-ib_0 \eta_1 \eta_2 / 2} e^{ib_0 \phi(\underline{y}, \eta)} \psi(\mathbf{k}, \underline{y}) d\mathbf{k}. \quad (2.5.2)$$

Assume that T is a bounded operator on $L^2(\mathbb{R}^2)$ with a jointly continuous integral kernel $T(\mathbf{x}; \mathbf{x}')$ for which there exists $\alpha, C > 0$ such that

$$|T(\mathbf{x}; \mathbf{x}')| \leq C e^{-\alpha \|\mathbf{x} - \mathbf{x}'\|}, \quad \forall \mathbf{x}, \mathbf{x}' \in \mathbb{R}^2.$$

We also assume that T commutes with the magnetic translations (2.5.1) which leads to (see also (2.4.6))

$$T(\mathbf{x}; \mathbf{x}') = e^{ib_0 \phi(\mathbf{x}, \eta)} T(\mathbf{x} - \eta; \mathbf{x}' - \eta) e^{-ib_0 \phi(\mathbf{x}', \eta)}, \quad \forall \eta \in \mathbb{Z}_{(q)}^2,$$

or, by replacing \mathbf{x}' with $\underline{y} + \eta$ and \mathbf{x} by $\underline{x} + \gamma$,

$$T(\underline{x} + \gamma; \underline{y} + \eta) = e^{ib_0 \phi(\gamma, \eta)} e^{ib_0 \phi(\underline{x}, \eta)} T(\underline{x} + \gamma - \eta; \underline{y}) e^{-ib_0 \phi(\underline{y}, \eta)}, \quad \forall \underline{x}, \underline{y} \in \Omega_{(q)}.$$

Then a straightforward computation shows that $\mathcal{U}_{BF} T \mathcal{U}_{BF}^*$ is a fibered operator $\int_{\mathbb{B}_{(q)}}^{\oplus} t_{\mathbf{k}} d\mathbf{k}$ where $t_{\mathbf{k}}$ is bounded on $L^2(\Omega_{(q)})$ and has the jointly continuous integral kernel

$$t_{\mathbf{k}}(\underline{x}; \underline{y}) := \sum_{\eta \in \mathbb{Z}_{(q)}^2} e^{-i\mathbf{k} \cdot \eta} e^{-ib_0 \eta_1 \eta_2 / 2} e^{-ib_0 \phi(\underline{x}, \eta)} T(\underline{x} + \eta; \underline{y}), \quad \forall \underline{x}, \underline{y} \in \Omega_{(q)}. \quad (2.5.3)$$

We observe that the above kernel is $\mathbb{Z}_{(q)}^{2*}$ periodic in \mathbf{k} and its Fourier coefficients give us back the original kernel:

$$T(\underline{x} + \eta; \underline{y}) = \frac{1}{|\mathbb{B}_{(q)}|} \int_{\mathbb{B}_{(q)}} t_{\mathbf{k}}(\underline{x}; \underline{y}) e^{i\mathbf{k} \cdot \eta} e^{ib_0 \eta_1 \eta_2 / 2} e^{ib_0 \phi(\underline{x}, \eta)} d\mathbf{k}, \quad \forall \underline{x}, \underline{y} \in \Omega_{(q)}.$$

In particular:

$$\frac{1}{|\Omega_{(q)}|} \int_{\Omega_{(q)}} T(\underline{x}; \underline{x}) d\underline{x} = \frac{1}{4\pi^2} \int_{\mathbb{B}_{(q)}} \left(\int_{\Omega_{(q)}} t_{\mathbf{k}}(\underline{x}; \underline{x}) d\underline{x} \right) d\mathbf{k}. \quad (2.5.4)$$

Most importantly, if T is an orthogonal projection like Π_b in (2.4.6) with $b = b_0$, then its corresponding fiber denoted by $p_{\mathbf{k}}$ is also an orthogonal projection, real analytic and periodic in \mathbf{k} , with finite (and constant) rank, and (2.5.4) can be restated as:

$$\lim_{L \rightarrow \infty} \frac{1}{|\Lambda_L|} \text{Tr}_{L^2(\mathbb{R}^2)}(\chi_L \Pi_{b_0}) = \frac{1}{4\pi^2} \int_{\mathbb{B}_{(q)}} \text{Tr}_{L^2(\Omega_{(q)})}(p_{\mathbf{k}}) d\mathbf{k} = \frac{\text{rank}(p)}{q} \in \mathbb{Q}. \quad (2.5.5)$$

Next we study the operator

$$T = i \Pi_{b_0} [[X_1, \Pi_{b_0}], [X_2, \Pi_{b_0}]]$$

which appears in (2.4.8). The commutators $[X_j, \Pi_{b_0}]$ have kernels given by $(x_j - x'_j) \Pi_{b_0}(\mathbf{x}; \mathbf{x}')$ and thus they are exponentially localized around the diagonal and commute with the magnetic translations. Let us find the fiber of $[X_j, \Pi_{b_0}]$.

Denote by U^Z the fibered unitary operator acting on $\int_{\mathbb{B}_{(q)}}^{\oplus} L^2(\Omega_{(q)}) d\mathbf{k}$ given by the fiber

$$(u_{\mathbf{k}}^Z \psi)(\underline{x}) := e^{-i\mathbf{k} \cdot \underline{x}} \psi(\underline{x}), \quad \forall \psi \in L^2(\Omega_{(q)}).$$

The Zak modification of the Bloch–Floquet unitary is $\mathcal{U}_{\text{BFZ}} := U^Z \mathcal{U}_{\text{BF}}$, and it will be called the Bloch–Floquet–Zak (BFZ) transform. The integral kernel of the BFZ transform applied to Π_{b_0} can be read off from (2.5.3):

$$p_{\mathbf{k}}^Z(\underline{x}; \underline{y}) := \sum_{\eta \in \mathbb{Z}_{(q)}^2} e^{-i\mathbf{k} \cdot (\underline{x} + \eta - \underline{y})} e^{-ib_0 \eta_1 \eta_2 / 2} e^{-ib_0 \phi(\underline{x}, \eta)} \Pi_{b_0}(\underline{x} + \eta; \underline{y}), \quad \forall \underline{x}, \underline{y} \in \Omega_{(q)}.$$

Differentiating with respect to k_j and conjugating back with $(u_{\mathbf{k}}^Z)^*$ we obtain that the fiber of $[X_j, \Pi_{b_0}]$ in the Bloch–Floquet representation is

$$(u_{\mathbf{k}}^Z)^* i (\partial_{k_j} p_{\mathbf{k}}^Z) u_{\mathbf{k}}^Z.$$

Thus the Bloch–Floquet fiber of T becomes

$$t_{\mathbf{k}} = -i p_{\mathbf{k}} (u_{\mathbf{k}}^Z)^* [\partial_{k_1} p_{\mathbf{k}}^Z, \partial_{k_2} p_{\mathbf{k}}^Z] u_{\mathbf{k}}^Z.$$

Introducing this into (2.5.4) and using trace cyclicity we obtain

$$\int_{\Omega} T(\mathbf{x}; \mathbf{x}) d\mathbf{x} = \frac{1}{|\Omega_{(q)}|} \int_{\Omega_{(q)}} T(\underline{x}; \underline{x}) d\underline{x} = -\frac{i}{4\pi^2} \int_{\mathbb{B}_{(q)}} \text{Tr}_{L^2(\Omega_{(q)})}(p_{\mathbf{k}}^Z [\partial_{k_1} p_{\mathbf{k}}^Z, \partial_{k_2} p_{\mathbf{k}}^Z]) d\mathbf{k}.$$

Thus

$$2\pi \lim_{L \rightarrow \infty} \frac{1}{|\Lambda_L|} \text{Tr}_{L^2(\mathbb{R}^2)}(\chi_L T) = \frac{1}{2\pi i} \int_{\mathbb{B}_{(q)}} \text{Tr}_{L^2(\Omega_{(q)})}(p_{\mathbf{k}}^Z [\partial_{k_1} p_{\mathbf{k}}^Z, \partial_{k_2} p_{\mathbf{k}}^Z]) d\mathbf{k} =: C(p^Z).$$

After an elementary but long computation one may show that

$$\begin{aligned} & \text{Tr}_{L^2(\Omega_{(q)})}(p_{\mathbf{k}}^Z dp_{\mathbf{k}}^Z \wedge dp_{\mathbf{k}}^Z) - \text{Tr}_{L^2(\Omega_{(q)})}(p_{\mathbf{k}} dp_{\mathbf{k}} \wedge dp_{\mathbf{k}}) \\ &= d \left\{ \text{Tr}_{L^2(\Omega_{(q)})}(p_{\mathbf{k}} (u_{\mathbf{k}}^Z)^* \wedge du_{\mathbf{k}}^Z) \right\}. \end{aligned}$$

The right hand side is periodic in \mathbf{k} , therefore after integration on the Brillouin zone and an application of Stokes' Theorem we obtain that $C(p^Z) = C(p)$. The latter is

well known to be an integer from the theory of vector bundles: for a direct proof (showing that it equals the winding number of the determinant of a certain smooth and 2π -periodic unitary matrix), see Proposition 5.5.3. More about the number $C(p^Z)$ can be found e.g. in [89].

In particular, when $C(p) = 0$ we may find (see Chapter 5) an orthonormal basis $\{\xi_j(\mathbf{k}, y)\}_{j \in J}$, where $J = \{1, \dots, \text{rank}(p)\}$, in the range of $p_{\mathbf{k}}$ which consists of real analytic vectors in \mathbf{k} and which are also periodic. Applying the inverse Bloch–Floquet transform as in (2.5.2) we obtain exponentially localized Wannier vectors

$$w_j(\underline{y} + \eta) := \frac{1}{|\mathbb{B}_{(q)}|^{1/2}} \int_{\mathbb{B}_{(q)}} e^{i\mathbf{k} \cdot \eta} e^{-ib_0 \eta_1 \eta_2 / 2} e^{ib_0 \phi(y, \eta)} \xi_j(\mathbf{k}, \underline{y}) d\mathbf{k}, \quad \underline{y} \in \Omega_{(q)}, \quad \eta \in \mathbb{Z}_{(q)}^2,$$

such that

$$\begin{aligned} \Pi_{b_0}(\mathbf{x}; \mathbf{x}') &= \sum_{j=1}^{\text{rank}(p)} \sum_{\gamma \in \mathbb{Z}_{(q)}^2} (\widehat{\tau}_{b_0, \gamma} w_j)(\mathbf{x}) \overline{(\widehat{\tau}_{b_0, \gamma} w_j)(\mathbf{x}')} \\ &= \sum_{j=1}^{\text{rank}(p)} \sum_{\gamma \in \mathbb{Z}_{(q)}^2} (\tau_{b_0, \gamma} w_j)(\mathbf{x}) \overline{(\tau_{b_0, \gamma} w_j)(\mathbf{x}')}. \end{aligned}$$

Notice that the above is exactly in the form (2.4.11) in the statement of Corollary 2.4.2.

2.5.2 Kernel regularity, exponential localization and gauge covariant magnetic perturbation theory

In this appendix we sketch the main ideas behind the estimates (2.4.21) and (2.4.36) and collect all the regularity results on integral kernels that we have used in the proofs, directly or indirectly. We only focus on (2.4.36) because (2.4.21) is nothing but (2.4.36) when the magnetic field perturbation vanishes.

Assume that the total magnetic field is given by $b + B_\lambda(\mathbf{x})$ where

$$\sup_{\mathbf{x} \in \mathbb{R}^2} |\partial^\alpha B_\lambda(\mathbf{x})| \leq \lambda^{|\alpha|+1} C_\alpha, \quad \alpha \in \mathbb{N}^2, \quad |\alpha| \leq 1.$$

Define the family of vector potentials depending on the parameter $\mathbf{y} \in \mathbb{R}^2$:

$$\mathcal{A}_\lambda(\mathbf{x}, \mathbf{y}) := \left(\int_0^1 s B_\lambda(\mathbf{y} + s(\mathbf{x} - \mathbf{y})) ds \right) (-x_2 + y_2, x_1 - y_1).$$

We have the estimates

$$|\partial_{\mathbf{x}}^\alpha \mathcal{A}_\lambda(\mathbf{x}, \mathbf{y})| \leq \lambda^{|\alpha|+1} C_\alpha \|\mathbf{x} - \mathbf{y}\|, \quad \alpha \in \mathbb{N}^2, \quad |\alpha| \leq 1. \quad (2.5.6)$$

It turns out that they all generate the same magnetic field $B_\lambda(\mathbf{x})$. Denote by $\mathcal{A}_\lambda(\mathbf{x}) := \mathcal{A}_\lambda(\mathbf{x}, \mathbf{0})$, as in (2.4.17). Then we must have that $\mathcal{A}_\lambda(\mathbf{x})$ and $\mathcal{A}_\lambda(\mathbf{x}, \mathbf{y})$ differ by a gradient, and one can show that

$$\mathcal{A}_\lambda(\mathbf{x}) - \mathcal{A}_\lambda(\mathbf{x}, \mathbf{y}) = \nabla_{\mathbf{x}} \phi_\lambda(\mathbf{x}, \mathbf{y})$$

where $\phi_\lambda(\mathbf{x}, \mathbf{y})$ is nothing but the magnetic phase defined in (2.4.35).

An identity which plays a fundamental role in the gauge covariant magnetic perturbation theory is

$$(\mathbf{P}_{\mathbf{x}} - \mathcal{A}_\lambda(\mathbf{x}))e^{i\phi_\lambda(\mathbf{x}, \mathbf{y})} = e^{i\phi_\lambda(\mathbf{x}, \mathbf{y})}(\mathbf{P}_{\mathbf{x}} - \mathcal{A}_\lambda(\mathbf{x}, \mathbf{y})), \quad \mathbf{P}_{\mathbf{x}} := -i\nabla_{\mathbf{x}}. \quad (2.5.7)$$

For the constant magnetic field b we introduce the linear magnetic potential $b\mathbf{A}(\mathbf{x}) = \frac{b}{2}(-x_2, x_1)$ with magnetic phase $b\phi(\mathbf{x}, \mathbf{x}')$ (see (2.4.4)), and we have the identity

$$(\mathbf{P}_{\mathbf{x}} - b\mathbf{A}(\mathbf{x}))e^{ib\phi(\mathbf{x}, \mathbf{y})} = e^{ib\phi(\mathbf{x}, \mathbf{y})}(\mathbf{P}_{\mathbf{x}} - b\mathbf{A}(\mathbf{x} - \mathbf{y})). \quad (2.5.8)$$

Let us recall a general result about the resolvent of any magnetic Schrödinger operator $H = \frac{1}{2m}(\mathbf{P} - \mathbf{a})^2 + V$ with a bounded magnetic field (the magnetic potential may grow) and a bounded electric potential, not necessarily periodic. Let $K \subset \rho(H)$ be a compact subset of the resolvent set of H . Then there exist two constants $\alpha, C > 0$ such that for every $z \in K$ the resolvent $(H - z)^{-1}$ has an integral kernel $(H - z)^{-1}(\mathbf{x}; \mathbf{x}')$ which is continuous outside the diagonal $\mathbf{x} = \mathbf{x}'$ and moreover [104, 19]

$$\sup_{z \in K} \left| (H - z\mathbf{1})^{-1}(\mathbf{x}; \mathbf{x}') \right| \leq C \ln \left(2 + \|\mathbf{x} - \mathbf{x}'\|^{-1} \right) e^{-\alpha\|\mathbf{x} - \mathbf{x}'\|}, \quad \forall \mathbf{x} \neq \mathbf{x}' \in \mathbb{R}^2. \quad (2.5.9)$$

This shows that the resolvent's kernel behaves like the one of the free Laplace operator in two dimensions. The constants α and C can be chosen to be independent of the magnitude of the magnetic field due to the diamagnetic inequality. The exponential decay is a consequence of Combes–Thomas estimates [26, 37].

In the case of a purely magnetic Landau operator $H_{\text{Landau}} := \frac{1}{2m}(\mathbf{P} - b\mathbf{A})^2$ its resolvent admits an explicit kernel of the type

$$(H_{\text{Landau}} + 1)^{-1}(\mathbf{x}; \mathbf{x}') = e^{ib\phi(\mathbf{x}, \mathbf{x}')} F(\|\mathbf{x} - \mathbf{x}'\|)$$

where F decays exponentially at infinity (it is in fact a Gaussian if $b \neq 0$) and has a local logarithmic singularity, see [36]. Also, using (2.5.8) one can show that there exist $\alpha, C > 0$ such that

$$\left| \{ (\mathbf{P}_{\mathbf{x}} - b\mathbf{A}(\mathbf{x})) (H_{\text{Landau}} + 1)^{-1}(\mathbf{x}; \mathbf{x}') \} \right| \leq C \|\mathbf{x} - \mathbf{x}'\|^{-1} e^{-\alpha\|\mathbf{x} - \mathbf{x}'\|}, \quad \forall \mathbf{x} \neq \mathbf{x}' \in \mathbb{R}^2. \quad (2.5.10)$$

We are interested in the integral kernel of the resolvents of

$$H_\lambda = \frac{1}{2m}(\mathbf{P} - b\mathbf{A} - \mathcal{A}_\lambda)^2 + V, \quad H_0 = \frac{1}{2m}(\mathbf{P} - b\mathbf{A})^2 + V.$$

Without loss of generality we may assume that the spectrum of H_0 is non-negative. The second resolvent identity

$$(H_0 + 1)^{-1} = (H_{\text{Landau}} + 1)^{-1} - (H_{\text{Landau}} + 1)^{-1}V(H_0 + 1)^{-1},$$

together with (2.5.9), (2.5.10) and the fact that V is bounded, lead to the existence of $\alpha, C > 0$ such that

$$\left| (\mathbf{P}_{\mathbf{x}} - b\mathbf{A}(\mathbf{x}))(H_0 + 1)^{-1}(\mathbf{x}; \mathbf{x}') \right| \leq C \|\mathbf{x} - \mathbf{x}'\|^{-1} e^{-\alpha\|\mathbf{x} - \mathbf{x}'\|}, \quad \forall \mathbf{x} \neq \mathbf{x}' \in \mathbb{R}^2. \quad (2.5.11)$$

Now if K is some compact set in $\rho(H_0)$ and $z \in K$, then from the first resolvent identity

$$(H_0 - z)^{-1} = (H_0 + 1)^{-1} + (z + 1)(H_0 + 1)^{-1}(H_0 - z)^{-1}$$

together with (2.5.9) and (2.5.11) we conclude that there exist $\alpha, C > 0$ such that

$$\sup_{z \in K} \left| (\mathbf{P}_{\mathbf{x}} - b\mathbf{A}(\mathbf{x}))(H_0 - z)^{-1}(\mathbf{x}; \mathbf{x}') \right| \leq C \|\mathbf{x} - \mathbf{x}'\|^{-1} e^{-\alpha \|\mathbf{x} - \mathbf{x}'\|}, \quad \forall \mathbf{x} \neq \mathbf{x}' \in \mathbb{R}^2. \quad (2.5.12)$$

We are now ready to deal with the magnetic perturbation induced by \mathcal{A}_λ . If $z \in \rho(H_0)$ we define the operator $S_\lambda(z)$ given by the integral kernel

$$S_\lambda(z)(\mathbf{x}; \mathbf{x}') := e^{i\phi_\lambda(\mathbf{x}, \mathbf{x}')} (H_0 - z)^{-1}(\mathbf{x}; \mathbf{x}'). \quad (2.5.13)$$

From (2.5.9) we see that $|S_\lambda(z)(\mathbf{x}; \mathbf{x}')|$ is pointwise bounded by a function of $\mathbf{x} - \mathbf{x}'$ which is in $L^1(\mathbb{R}^2)$, thus via Schur's criterion $S_\lambda(z)$ defines a bounded operator. The main observation is that the range of $S_\lambda(z)$ lies in the domain of $H_\lambda - z$ and using (2.5.7) we have

$$(H_\lambda - z)S_\lambda(z) =: \mathbf{1} + T_\lambda(z) \quad (2.5.14)$$

where $T_\lambda(z)$ has an integral kernel given by

$$\begin{aligned} T_\lambda(z)(\mathbf{x}; \mathbf{x}') &:= -2e^{i\phi_\lambda(\mathbf{x}, \mathbf{x}')} \mathcal{A}_\lambda(\mathbf{x}, \mathbf{x}') \cdot (\mathbf{P}_{\mathbf{x}} - b\mathbf{A}(\mathbf{x}))(H_0 - z)^{-1}(\mathbf{x}; \mathbf{x}') \\ &\quad + e^{i\phi_\lambda(\mathbf{x}, \mathbf{x}')} \left\{ |\mathcal{A}_\lambda(\mathbf{x}, \mathbf{x}')|^2 - i \operatorname{div}_{\mathbf{x}} \mathcal{A}_\lambda(\mathbf{x}, \mathbf{x}') \right\} (H_0 - z)^{-1}(\mathbf{x}; \mathbf{x}'). \end{aligned}$$

From this formula we see, by using (2.5.6), (2.5.9) and (2.5.12), that $|T_\lambda(z)(\mathbf{x}; \mathbf{x}')|$ is also bounded by an $L^1(\mathbb{R}^2)$ -function of $\mathbf{x} - \mathbf{x}'$, namely

$$|T_\lambda(z)(\mathbf{x}; \mathbf{x}')| \leq C \lambda e^{-\alpha \|\mathbf{x} - \mathbf{x}'\|}. \quad (2.5.15)$$

The factor λ ensures that $\|T_\lambda(z)\| \leq C \lambda < 1$ uniformly in $z \in K$ if λ is small enough. Hence we have that $H_\lambda - z$ is invertible and

$$(H_\lambda - z)^{-1} = S_\lambda(z) \{ \mathbf{1} + T_\lambda(z) \}^{-1}.$$

Multiplying both sides of (2.5.14) by $(H_\lambda - z)^{-1}$ then yields a resolvent-like identity:

$$(H_\lambda - z)^{-1} = S_\lambda(z) - (H_\lambda - z)^{-1} T_\lambda(z). \quad (2.5.16)$$

We have just proved that the gaps in the spectrum of H_0 are stable. Thus if σ_0 is an isolated spectral island of H_0 and $\mathcal{C} \subset \rho(H_0)$ is a positively oriented simple contour which encircles σ_0 , then \mathcal{C} also belongs to $\rho(H_\lambda)$ if λ is small enough and we can define two Riesz projections as

$$\Pi_\lambda = \frac{i}{2\pi} \oint_{\mathcal{C}} (H_\lambda - z)^{-1} dz, \quad \Pi_0 = \frac{i}{2\pi} \oint_{\mathcal{C}} (H_0 - z)^{-1} dz.$$

Using (2.5.9) and the identities $\Pi_\lambda = \Pi_\lambda^2$ and $\Pi_0 = \Pi_0^2$ one can show that the integral kernels of both projections are no longer singular and, at the same time, they have an exponential localization near the diagonal, see also Appendix A.1 for more details. Moreover, by applying the Riesz integral to (2.5.16), using the explicit expression (2.5.13) for $S_\lambda(z)(\mathbf{x}; \mathbf{x}')$, and noting that

$$\sup_{z \in \mathcal{C}} \left| \{ (H_\lambda - z)^{-1} T_\lambda(z) \}(\mathbf{x}; \mathbf{x}') \right| \leq C \lambda e^{-\alpha \|\mathbf{x} - \mathbf{x}'\|}$$

from (2.5.15), we finish the proof of (2.4.36).

Chapter 3

A case study: ultra generalized Wannier functions

In Chapter 1 we gave a definition of generalized Wannier basis and in Chapter 2 we generalized the concept of Chern number by means of position-space objects. In this chapter we show that relaxing the concept of generalized Wannier functions permits to construct a large number of different types of generalized Wannier basis. However, at the same time we provide an explicit example that evidences how this new objects are not capable to encode the transport properties of physical systems. We review and extend the Prodan's construction of radially localized generalized Wannier basis, that hereafter are called Ultra Generalized Wannier basis (UGWB), for Hamiltonian operators that satisfy Assumption 1.3.3. After that we explicitly construct a ultra generalized Wannier basis for the lowest Landau level. The results in this chapter are a joint work with G. Panati.

3.1 Prodan's ultra generalized Wannier basis

As we recalled in Chapter 1 the construction of a generalized Wannier basis in dimension $d = 1$ is based on the spectral theory of the reduced position operator $\tilde{X} = P_\mu X P_\mu$. In particular, the eigenvalues and eigenvectors of \tilde{X} are interpreted as points of a (not necessarily regular) lattice and, respectively, generalized Wannier functions for the spectral projection P_μ . As it is well known, the operator X is an unbounded operator whose spectrum is purely absolutely continuous and covers the entire real line \mathbb{R} . However, the projection of the action of X onto the spectral subspace associated to P_μ gives the chance to create discrete spectrum. Indeed, by definition of discrete spectrum, $\varphi \in L^2(\mathbb{R}^2)$ is an eigenvector for X if and only if φ is in the kernel of $(X - \lambda)$ with $\lambda \in \mathbb{R}$, that is

$$(X - \lambda)\varphi = 0.$$

Clearly the kernel of $(X - \lambda)$ contains only the zero vector. Consider now the eigenvalue equation for \tilde{X} . Since $P_\mu^2 = P_\mu$, we have that $\varphi \in P_\mu L^2(\mathbb{R}^2)$ is an eigenvector for \tilde{X} if and only if φ is in the kernel of $P_\mu (X - \lambda) P_\mu$. Because of the infinite dimension of the kernel of P_μ , in principle it is possible to find an infinite

number of eigenvectors. This is exactly what happens in the $d = 1$ case. Therefore, in the range of P_μ , it is logical to interpret the eigenvalues of \tilde{X} as points in the space, since

$$XP_\mu\varphi = \lambda P_\mu\varphi + \varphi_\perp$$

where $P_\mu\varphi_\perp = 0$. This fundamental idea is behind both the construction of the one-dimensional generalized Wannier basis and the ultra generalized Wannier basis. Notice that the same argument holds true if we consider $f(X)$ in place of X . However, it is necessary for f to be invertible in order to recover a true lattice from the spectrum of the operator $f(X)$.

We showed in Chapter 1 that in $d > 1$ the operator $P_\mu X_i P_\mu$ is not necessarily compact. However, if one considers $f(X)$ instead of X_i it is possible to overcome the compactness problem. This is exactly the key idea in the paper by Prodan [96]. In the following we extend the Prodan's construction also for systems that are not time-reversal symmetric. We present here the results for $d = 2$, however the proof can be easily extended in the same way to $d > 2$.

Theorem 3.1.1 (Generalization of [96]). *Consider a Hamiltonian operator H satisfying Assumption 1.3.3. For $q > 0$, let W_q be the following bounded, selfadjoint operator*

$$W_q : P_\mu\mathcal{H} \rightarrow P_\mu\mathcal{H}, \quad W_q := P_\mu e^{-q\langle X \rangle} P_\mu. \quad (3.1.1)$$

Then:

- (i) W_q is a compact operator, hence its spectrum is discrete, of finite degeneracy, and has only one accumulation point at zero.
- (ii) Let $(\lambda_i, \{\psi_{i,j}(x)\}_{j \leq m_i < \infty})_{i \in \mathbb{N}}$ be the set of eigenpairs for W_q , with eigenvalues $\{\lambda_i\}_{i \in \mathbb{N}}$ ordered decreasingly. Define

$$\langle r_i \rangle := \frac{-\ln(\lambda_i)}{q}, \quad (3.1.2)$$

where the expression makes sense since all the eigenvalues are positive. Then, all the eigenvectors decay exponentially at infinity with a rate β and are radially localized in the sense that

$$\sup_{i,j} \int_{\mathbb{R}^2} e^{2\beta|\langle \mathbf{x} \rangle - \langle r_i \rangle|} |\psi_{i,j}(\mathbf{x})|^2 d\mathbf{x} \leq M < \infty, \quad (3.1.3)$$

with $|y|' = y$ if $y \geq 0$ and $|y|' = -\frac{1}{2}y$ if $y < 0$.

We call *ultra generalized Wannier basis* (UGWB) a basis for the range of P_μ with the radial localization property described in Theorem 3.1.1 (ii).

Remark 3.1.2. Note that it is not possible to construct a two-dimensional lattice using the spectrum of W_q . Nevertheless, it is possible to identify a sequence of concentric annuli where each Wannier function is concentrated in. Although on one hand this particular localization shape can be useful for some radially symmetric problems [96], on the other hand the radial localization clearly breaks the translation symmetry, that is, even in the case of a periodic system the ultra generalized Wannier basis cannot be built by acting with the symmetry translation group on a finite set of functions.

In order to prove Theorem 3.1.1 we need a technical lemma that is already present in the literature. For the sake of completeness we recall here the main steps of the proof. The lemma is about the relative compactness of operators with respect to a Hamiltonian operator, with and without magnetic field.

Lemma 3.1.3 ([7]). *Let H be as in the Assumption 1.3.3 and T be a positive multiplication operator and $E \in \mathbb{R}$. If $T(-\Delta + E)^{-1}$ is a compact operator, then also $T(-\Delta_A + E)^{-1}$ is a compact operator.*

The proof of Lemma 3.1.3 is an application of the Dodd–Fremlin–Pitt criterion of compactness. We write here the statement of the theorem, while the proof can be found in [95].

Theorem 3.1.4 (Dodd–Fremlin–Pitt criterion of compactness). *Consider two bounded operators T, S on the Hilbert space $\mathcal{H} = L^2(\mathbb{R}^n)$. We say that $T \stackrel{\leq}{\prec} S$ if, for every $\psi \in \mathcal{H}$ it holds that*

$$|T\psi(\mathbf{x})| \leq (S|\psi|)(\mathbf{x}) \quad \text{for a.e. } \mathbf{x} \in \mathbb{R}^n. \quad (3.1.4)$$

If S is a compact operator and $T \stackrel{\leq}{\prec} S$, then T is also a compact operator.

Proof of Lemma 3.1.3. By writing the resolvent as

$$(-\Delta_A + E)^{-1} = \int_0^\infty dt e^{-tE} e^{t\Delta_A} \quad (3.1.5)$$

and using the diamagnetic inequalities [104]

$$e^{t\Delta_A} \stackrel{\leq}{\prec} e^{t\Delta}, \quad (3.1.6)$$

one obtains

$$T(-\Delta_A + E)^{-1} \stackrel{\leq}{\prec} T(-\Delta + E)^{-1}. \quad (3.1.7)$$

Then [7, Theorem 2.2] guarantees that $T(-\Delta_A + E)^{-1}$ is a compact operator. \square

3.1.1 Proof of Theorem 3.1.1

The proof of Theorem 3.1.1 basically follows the argument of [96], with the exception of step (i) where the presence of the magnetic field has to be taken into account. The proof has two crucial ingredients. One is the diamagnetic inequality in the form of the Dodd–Fremlin–Pitt criterion and the other is the Combes–Thomas estimate.

(i) Thanks to the gap hypothesis, one may use the Riesz formula to obtain

$$W_q = P_\mu \frac{i}{2\pi} \oint_{\mathcal{C}} e^{-q\langle X \rangle} (H_A - z)^{-1} dz \quad (3.1.8)$$

where \mathcal{C} is a positively oriented curve surrounding the spectral island $\sigma_0(H_A)$. Since $-\Delta_A$ is bounded from below, see Proposition 1.3.5 with $V = 0$, there exists $a \in \mathbb{R}$ such that $(-\Delta_A + a)^{-1}$ is a bounded operator. Hence we have

$$W_q = P_\mu \frac{i}{2\pi} \oint_{\mathcal{C}} e^{-q\langle X \rangle} (-\Delta_A + a)^{-1} (-\Delta_A + a) (H_A - z)^{-1} dz. \quad (3.1.9)$$

As it is proved in [96], $e^{-q\langle X \rangle}(-\Delta + a)^{-1}$ is an operator of the form $f(X)g(P)$ with $f, g \in L^s(\mathbb{R}^2)$ for $s \geq 2$. In view of [1, Proposition 2.34], one concludes that $e^{-q\langle X \rangle}(-\Delta + a)^{-1}$ is an operator in the s -Schatten class [106] and hence compact. So we can apply Lemma 3.1.3 with $T = e^{-q\langle X \rangle}$ and conclude that also $e^{-q\langle X \rangle}(-\Delta_A + a)^{-1}$ is a compact operator.

Moreover

$$\begin{aligned} (-\Delta_A + a)(H_A - z)^{-1} &= (-\Delta_A + V - z - V + z + a)(H_A - z)^{-1} \\ &= 1 + (z + a)(H_A - z)^{-1} - V(H_A - z)^{-1}. \end{aligned}$$

The first two summands are bounded operators and $V(H_A - z)^{-1}$ is a bounded operator because V is relatively bounded w.r. to $-\Delta_A$, see Remark 1.3.4. Since the compact operators are a closed ideal in $\mathcal{B}(\mathcal{H})$, and the contour $\mathcal{C} \subset \mathbb{C}$ is compact, one concludes that that W_q is a compact operator.

- (ii) This part is the same as in [96]. Let ψ be a normalized eigenvector, $W_q\psi = \lambda\psi$. We have that, for any $q > 0$,

$$\lambda = \langle \psi, W_q\psi \rangle = \int_{\mathbb{R}^2} e^{-q\langle \mathbf{x} \rangle} |\psi(\mathbf{x})|^2 d\mathbf{x} \leq e^{-q} \|\psi\|^2 = e^{-q}. \quad (3.1.10)$$

In particular, this shows that $0 < \lambda < 1$. Consider now W_β , with β small enough such that we can apply the Combes–Thomas estimate (Proposition A.1.5) which together with Riesz formula implies

$$\left\| e^{\beta\langle X \rangle} P_\mu e^{-\beta\langle X \rangle} \right\| \leq C.$$

One notices that

$$\begin{aligned} \left[\int_{\mathbb{R}^2} e^{2\beta\langle \mathbf{x} \rangle} |\psi(\mathbf{x})|^2 d\mathbf{x} \right]^{\frac{1}{2}} &= \left\| e^{\beta\langle X \rangle} \psi \right\| \\ &= \lambda^{-1} \left\| e^{\beta\langle X \rangle} W_\beta \psi \right\| \\ &= \lambda^{-1} \left\| e^{\beta\langle X \rangle} P_\mu e^{-\beta\langle X \rangle} \psi \right\| \leq \lambda^{-1} C. \end{aligned} \quad (3.1.11)$$

Therefore the eigenfunctions of W_β decay exponentially at infinity with rate β .

- (iii) Since the eigenvalues λ_i are positive and accumulate at zero, $\{\langle r_i \rangle\}$ is a sequence of positive numbers which increase monotonically to infinity. Let ψ_i be the eigenvector relative to λ_i , then (3.1.11) becomes

$$\int_{\mathbb{R}^2} e^{2\beta(\langle \mathbf{x} \rangle - \langle r_i \rangle)} |\psi(\mathbf{x})|^2 d\mathbf{x} \leq C^2. \quad (3.1.12)$$

On the other hand

$$1 = \lambda^{-1} \langle \psi_i, W_\beta \psi_i \rangle = \int_{\mathbb{R}^2} e^{\beta(\langle r_i \rangle - \langle \mathbf{x} \rangle)} |\psi(\mathbf{x})|^2 d\mathbf{x}. \quad (3.1.13)$$

By defining $M = \max\{1, C^2\}$, we obtain the radial localization of the theorem.

Remark 3.1.5. At a first glance, it seems that there is some freedom in the choice of the multiplication operator which appears in the definition of W_q ; however there are - at least - two main constraints. First, as one can see from the proof of Theorem 3.1.1, the multiplication operator $e^{-q\langle \cdot \rangle}$ which defines W_q via (3.1.1) has to be in $L^s(\mathbb{R}^2)$ for some s in order to prove the compactness of W_q . Moreover, to prove an estimate similar to (3.1.11) the multiplication operator has to be related with the Combes–Thomas estimates theory. These two constraints together, heavily restrict the possible choices of multiplication operators that can be used to define W_q .

3.2 An explicit example: the Landau Hamiltonian

After having proved the existence of the ultra generalized Wannier basis in a general setting, it is a valid question to ask whether the UGWB is a merely mathematical artefact or it does carry some information about the transport properties of the solid modelled by the Hamiltonian operator H_A . In this regards, we now explicitly construct the UGWB for the lowest Landau level.

Consider the Landau Hamiltonian operator (LH), namely the Hamiltonian operator acting in $L^2(\mathbb{R}^2)$ and describing a point charge particle moving under the influence of a constant magnetic field perpendicular to the xy plane defined by

$$H_L := \frac{1}{2}(-i\nabla - b\mathbf{A}_L)^2, \quad (3.2.1)$$

where \mathbf{A}_L is the magnetic potential corresponding to a constant magnetic field in the symmetric gauge, that is $\mathbf{A}_L(\mathbf{x}) = \frac{1}{2}(-x_2, x_1)$. We set $b = \frac{q}{c}(\mathbf{B} \cdot \mathbf{e}_3)$, where q denotes the charge of the particle, c is the speed of light and \mathbf{B} is the uniform magnetic field. Up to an appropriate choice of the orthonormal frame, one can always assume that $b > 0$, as we do hereafter. Notice, however, that the dynamics depends on the sign of the charge, since for positive charges one has $(\mathbf{B} \cdot \mathbf{e}_3) > 0$, while $(\mathbf{B} \cdot \mathbf{e}_3) < 0$ for negative charges. H_L is essentially selfadjoint on the dense domain $C_0^\infty(\mathbb{R}^2)$ and its spectrum is discrete and given by

$$E_n = \frac{|b|}{2}(2n + 1), \quad n \in \mathbb{N}, \quad (3.2.2)$$

where each E_n is infinitely degenerate and it is called the n^{th} Landau level¹.

Each Landau level, and in particular the lowest Landau level (LLL) is unitarily equivalent to the Segal-Bargmann space [52]. This unitary equivalence provides a simple characterization of the vectors in the LLL and will be used to construct the explicit example of UGWB. Let us now briefly recall how to unitarily identify the two spaces. Define the following operators

$$\begin{aligned} K_1 &:= \frac{1}{b}(P_1 + \frac{b}{2}X_2), & K_2 &:= P_2 - \frac{b}{2}X_1; \\ G_1 &:= \frac{1}{b}(P_2 + \frac{b}{2}X_1), & G_2 &:= \frac{1}{b}(-P_1 + \frac{b}{2}X_2). \end{aligned} \quad (3.2.3)$$

¹With a little abuse of terminology, we use the term “ n^{th} Landau level” or “lowest Landau level” also to refer to the corresponding eigenspaces.

Note that the operators (G_1, G_2) are the quantum analogous of the coordinates of the cyclotron orbit in the classical theory. By a simple substitution, one can write the Hamiltonian as $H_L = \frac{1}{2}(K_2^2 + b^2 K_1^2)$. All the operators defined in (3.2.3) are essentially selfadjoint on $C_0^\infty(\mathbb{R}^2)$, see [58, Proposition 9.40], and by explicit computations one observes that they satisfy the following commutation relations

$$\begin{aligned} [K_1, K_2] &= i\mathbf{1}, & [G_1, G_2] &= -\frac{i}{b}\mathbf{1}, \\ [K_j, G_l] &= 0, & \forall j, l \in \{1, 2\}. \end{aligned} \quad (3.2.4)$$

Consider now the couple of ladder operators, namely

$$\begin{aligned} B &= \sqrt{\frac{b}{2}}(G_1 - iG_2) \\ B^* &= \sqrt{\frac{b}{2}}(G_1 + iG_2). \end{aligned}$$

One can easily check that $[B, B^*] = \mathbf{1}$. Mimicking the algebraic approach to the Hamiltonian of the harmonic oscillator, one can prove that the number operator B^*B has discrete spectrum and the role of the raising and lowering operators is played now by B^* and B respectively. A simple computation shows that the vector

$$\varphi_0(\mathbf{x}) = \left(\frac{b}{2\pi}\right)^{\frac{1}{2}} e^{-\frac{|b|}{4}\|\mathbf{x}\|^2} \quad (3.2.5)$$

is an eigenfunction for H_L with eigenvalue E_0 , namely φ_0 is in the LLL. By direct computation one can also check that the eigenfunction φ_0 defined in (3.2.5) satisfies

$$B\varphi_0 = 0.$$

This means that φ_0 is in the kernel of the number operator B^*B . Since the operators G_i commute with the operators K_i , we have that

$$H_L(B^*)^n\varphi_0 = (B^*)^n H_L\varphi_0 = 0.$$

Therefore all the infinite eigenvectors of the number operator B^*B are eigenvectors of H_L corresponding to the lowest Landau level. Since B^*B is a selfadjoint operator, eigenvectors corresponding to different eigenvalues are orthogonal.

The previous discussion shows that the LLL can be constructed using only the operator B and B^* . Explicitly, B acts as

$$(B\psi)(x, y) = \sqrt{\frac{1}{2b}} \left(\frac{\partial\psi}{\partial x_1}(x, y) - i \frac{\partial\psi}{\partial x_2}(x, y) + \frac{b}{2}(x_1 - ix_2)\psi(x, y) \right), \forall \psi \in C_0^\infty(\mathbb{R}^2).$$

Identifying \mathbb{R}^2 with the complex plane, namely $x_1 + ix_2 =: z \in \mathbb{C}$, and setting

$$\partial := \frac{1}{2} \frac{\partial}{\partial z} = \frac{1}{2} \left(\frac{\partial}{\partial x_1} - i \frac{\partial}{\partial x_2} \right), \quad \bar{\partial} := \frac{1}{2} \frac{\partial}{\partial \bar{z}} = \frac{1}{2} \left(\frac{\partial}{\partial x_1} + i \frac{\partial}{\partial x_2} \right),$$

we have that

$$B\psi(z) = \sqrt{\frac{1}{2b}} \left(2\partial + \frac{b}{2}\bar{z} \right) \psi(z)$$

and similarly

$$B^* \psi(z) = \sqrt{\frac{1}{2b}} \left(-2\bar{\partial} + \frac{b}{2}z \right) \psi(z).$$

If we substitute ψ with the eigenvector φ_0 defined in (3.2.5), we get that

$$B\varphi_0(z) = 0, \quad B^*\varphi_0(z) = \sqrt{\frac{b}{2}} z\varphi_0(z).$$

This means that the action of the raising operator B^* on φ_0 amounts to multiplication by z . Therefore, since the LLL is a closed subspace, we get that a generic function in the LLL is of the form

$$\psi(z) = f(z)\varphi_0(z)$$

where $f(z)$ is analytic and such that

$$\int_{\mathbb{C}} dz |f(z)|^2 |\varphi_0(z)|^2 < \infty.$$

From the commutation relation $[B, B^*] = \mathbf{1}$ one can deduce that the action of B and B^* can be described only in terms of the analytic function f , that is

$$(Bf\varphi_0)(z) = \sqrt{\frac{2}{b}} (\partial f(z)) \varphi_0(z), \quad (B^*f\varphi_0)(z) = \sqrt{\frac{b}{2}} z f(z) \varphi_0(z).$$

To be more precise, one considers the Gaussian measure $d\mu := N e^{-\frac{|b|}{4}|z|^2} dz$, with N positive constant, and defines the weighted L^2 -space

$$L^2(\mathbb{C}, d\mu) := \left\{ g : \mathbb{C} \rightarrow \mathbb{C} : \int_{\mathbb{C}} |g(z)|^2 d\mu < \infty \right\}$$

endowed with the scalar product

$$\langle f, g \rangle_{SB} := \int_{\mathbb{C}} \overline{f(z)} g(z) d\mu(z).$$

Definition 3.2.1 (Segal [103], Bargmann [11]). Let $\text{Hol}(\mathbb{C})$ be the space of entire functions. The Segal-Bargmann space $SB(\mathbb{C})$ is defined as

$$SB(\mathbb{C}) := \left\{ g \in \text{Hol}(\mathbb{C}) : \int_{\mathbb{C}} |g(z)|^2 d\mu(z) < \infty \right\} = L^2(\mathbb{C}, d\mu(z)) \cap \text{Hol}(\mathbb{C}).$$

It is straightforward to identify the LLL and the Segal-Bargmann space via the unitary operator $U : \Pi_0 L^2(\mathbb{R}^2) \rightarrow SB(\mathbb{C})$ defined by

$$(U\psi)(z) = f(z)$$

where $\psi(x, y) = f(x, y)\varphi_0(x, y)$, and Π_0 denotes the projection onto the LLL. Therefore we obtain

$$U\Pi_0 B \Pi_0 U^* = \sqrt{\frac{2}{b}} \partial, \quad U\Pi_0 B^* \Pi_0 U^* = \sqrt{\frac{b}{2}} z.$$

Notice that the operators G_i are related to the operator z and ∂ by the following relations

$$\begin{aligned} U\Pi_0(B + B^*)\Pi_0U^* &= U\Pi_0(\sqrt{2b}G_1)\Pi_0U^* = \sqrt{\frac{1}{2b}}(2\partial + bz) , \\ U\Pi_0(B^* - B)\Pi_0U^* &= U\Pi_0(i\sqrt{2b}G_2)\Pi_0U^* = \sqrt{\frac{1}{2b}}(bz - 2\partial) . \end{aligned} \quad (3.2.6)$$

We denote by P_0 the projection on $SB(\mathbb{C})$ acting in $L^2(\mathbb{C}, d\mu(z))$. Fix now $b = 4$, $N = \frac{1}{\pi}$, simply to recover the standard definition of Segal-Bargmann space.

An easy calculation shows that (3.2.1) satisfies Assumption 1.3.3, therefore a spectral projection onto any of the Landau level admits an UGWB in the sense of Theorem 3.1.1. Moreover, in this setting, the Prodan operator W_q is a particular restriction of a *Toeplitz operator* [117].

Definition 3.2.2 (Toeplitz operator). Let F be a bounded measurable function on the complex plane \mathbb{C} , and M_F the multiplication operator in $L^2(\mathbb{C}, d\mu(z))$ associated to the function F , that is $(M_Fg)(z) = F(z)g(z)$. The operator

$$T_F := P_0 M_F \quad (3.2.7)$$

is called Toeplitz operator associated to the symbol F .

If we take as P_μ in Theorem 3.1.1 the orthogonal projection on the LLL, so that $P_\mu = \Pi_0$, we have that W_q is unitarily equivalent to the restriction to $\text{Ran } P_0$ of the Toeplitz operator associated to the symbol $l(|z|) := e^{-q\sqrt{(1+|z|^2)}}$:

$$UW_qU^* = P_0 T_l P_0 . \quad (3.2.8)$$

Because of this particular structure, we are able to give an explicit formula both for the eigenfunctions and eigenvalues of the Prodan operator W_q in the special case of the Landau Hamiltonian operator. In particular this provides an explicit example of an ultra generalized Wannier basis in presence of magnetic field. The crucial result is given by the following theorem of Yoshino [117].

Theorem 3.2.3 (Yoshino [117]). *Let F be a bounded integrable and radial function over \mathbb{C} , i. e. $F(z) = \tilde{F}(|z|^2)$. Then the following statements hold:*

(i) *The functions $\{z^m\}_{m \in \mathbb{N}}$ are the eigenfunctions of T_F .*

(ii) *The eigenvalue λ_m of T_F , associated with the eigenfunction z^m is given by*

$$\lambda_m = \frac{1}{m!} \int_0^\infty \tilde{F}(s) e^{-s} s^m ds . \quad (3.2.9)$$

Proposition 3.2.4. *The ultra generalized Wannier basis associated to the lowest Landau level is given by the set $\{z^m\}_{m \in \mathbb{N}}$, and the corresponding eigenvalue λ_m are explicitly given by*

$$\lambda_m = \frac{1}{m!} \int_0^\infty e^{-q\sqrt{(1+s)}} e^{-s} s^m ds . \quad (3.2.10)$$

It is useful to obtain an estimate of $\langle r_m \rangle$ for this UGWB. We notice that

$$\lambda_m \leq \frac{e^{-q}}{m!} \int_0^\infty e^{-s} s^m ds = e^{-q} \frac{m!}{m!} = e^{-q}. \quad (3.2.11)$$

$$\lambda_m \geq \frac{1}{m!} \int_0^\infty e^{-q(1+\frac{s}{2})} e^{-s} s^m ds = \frac{e^{-q}}{m!} \int_0^\infty e^{-s(1+\frac{q}{2})} s^m ds. \quad (3.2.12)$$

Thus we get

$$\lambda_m \geq \frac{e^{-q}}{m!(1+\frac{q}{2})^{m+1}} \int_0^\infty e^{-s} s^m ds = e^{-q} (1+\frac{q}{2})^{-(m+1)}. \quad (3.2.13)$$

Summing up we obtain

$$1 \leq \langle r_m \rangle \leq 1 + (m+1) \ln(1+\frac{q}{2})^{\frac{1}{q}}. \quad (3.2.14)$$

It is also a well-known fact that every Landau level has a Quantum Hall conductivity, see for example [9], equal to $\frac{1}{2\pi}$, in natural units, hence the Chern character of Π_0 is different from zero, see for example Theorem 2.2.1. Therefore, Proposition 3.2.4 provides an explicit example of a UGWB for a system that is not time-symmetric and with non trivial topological features.

3.3 Conclusions

In this chapter we showed that the Prodan's construction [96] of ultra generalized Wannier basis can be extended to systems that are not time-reversal symmetric, provided that they satisfy the general Assumption 1.3.3 on the Hamiltonian operator. At a first look, this result seems to contradict the localization dichotomy paradigm of [79] and summarized in Section 1.2.4. Indeed, it is not difficult to exhibit an example of periodic gapped Hamiltonian satisfying Assumption 1.3.3 and such that the Chern number associated to the isolated spectral island is non-zero. In fact, by means of the simple example of the Landau Hamiltonian operator, we explicitly proved that one can construct an ultra generalized Wannier basis even for systems that are not topologically trivial, in the sense that their Chern character, defined in Definition 2.1.3, is non-zero. Choosing the magnetic field b such that it satisfies the rationality condition of Section 1.2.2 shows that one can construct an UGWB when the usual Chern number (5.3.2) is non-zero. Therefore, this result shows that, contrary to a composite Wannier basis, an ultra generalized Wannier basis does not encode transport or topological information about the physical system.

As we already pointed out before, the UGWB for a periodic system has the problem that it is not translation invariant, namely it does not have a ladder structure like the usual Wannier basis. We believe that this is the reason why the UGWB is not able to grasp the topological and transport properties of the system. We are aware that the last claim is not a true theorem and future work is planned to substantiate this claim on a solid mathematical background.

Chapter 4

Localization implies topological triviality

The decay properties in position space of the Wannier functions spanning a Fermi projection are tightly related to the topological properties of the Bloch bundle structure associated to the same projection. This paradigm is substantiated in a precise form by the localization dichotomy proved in [79] and summarized in Section 1.2.4.

In the previous chapters we paved the way to the generalization of Theorem 1.2.18 to the non periodic case. Indeed, in Chapter 1 we gave a clear definition of generalized Wannier basis, then in Chapter 2 we explained how it is possible to extend the notion of topological triviality in the disordered case. Finally, in Chapter 3 we showed, by means of an explicit example, that the definition of generalized Wannier basis has, to some extent, a rigid structure, in particular if one want to extract from it information concerning the transport properties of the system.

In this chapter we state a precise conjecture about the generalization of Theorem 1.2.18 to non periodic gapped systems and then we provide a proof for the first part of the conjecture. Specifically, we show that the existence of a “well” localized generalized Wannier basis for the projection P_μ implies the vanishing of the Chern character of P_μ . The work presented in this chapter is a fruit of a joint collaboration with G. Marcelli and G. Panati.

4.1 The Localization Dichotomy conjecture

Consider a Hamiltonian operator H satisfying Assumption 1.3.3. Then, the spectrum $\sigma(H)$ has a spectral island $\sigma_0(H)$ and P_μ is the projection onto $\sigma_0(H)$. In view of the results of the previous chapters we are now ready to state a well-posed conjecture on the generalization of Theorem 1.2.18 to the non periodic case. Recall that the generalized Wannier basis and the Chern character have been defined in Definition 1.3.6 and Definition 2.1.3 respectively.

Theorem 4.1.1 (Localization dichotomy conjecture). *Let P_μ be the spectral projection onto the spectral island $\sigma_0(H)$ of a gapped Hamiltonian H satisfying Assumption 1.3.3. Then the following statements are equivalent*

- (a) P_μ admits a generalized Wannier basis that is exponentially localized.
- (b) P_μ admits a generalized Wannier basis that is s -localized with $s = s^*$.
- (c) P_μ is topologically trivial in the sense that its Chern character $C(P_\mu)$ exists and is equal to zero.

As we have already mentioned before, (a) implies (b) by a simple inequality. In view of the argument in Section 2.3, proving that (c) implies (a) would solve the Nenciu's conjecture about the existence of generalized Wannier bases for time-reversal symmetric systems. In the next section, we prove that (b) with $s^* > 5$ implies (c). Clearly the result does not seem optimal. In fact, a true generalization of Theorem 1.2.18 would require to have $s^* = 1$. However, we believe that in order to reach $s^* = 1$ it is necessary to require stricter hypothesis on the potentials in Assumption 1.3.3. Further work in this direction is planned for the future.

4.2 Main result

Recall the definition of generalized Wannier basis, Definition 1.3.6, and define the set $\mathcal{M} := \cup_{\gamma \in \mathfrak{D}} (\{\gamma\} \times \{1, \dots, m(\gamma)\})$. Note that, by definition of GWB, there exists $m^* > 0$ such that $m^* > m(\gamma)$ for all $\gamma \in \mathfrak{D}$. Let us summarize our result in the following theorem.

Theorem 4.2.1 (Localization implies topological triviality). *Suppose that P_μ admits a s -localized generalized Wannier basis, $\{\psi_{\gamma,a}\}_{(\gamma,a) \in \mathcal{M}}$ for all $s \geq s^* > 5$, that is*

$$\int_{\mathbb{R}^2} |\psi_{\gamma,a}(\mathbf{x})|^2 (1 + \|\mathbf{x} - \gamma\|^2)^s d\mathbf{x} \leq M_s.$$

Then the Chern character of P_μ is zero, namely

$$\mathcal{T}(iP_\mu [[X_1, P_\mu], [X_2, P_\mu]]) = 0, \quad (4.2.1)$$

where \mathcal{T} is the trace per unit volume and X_1 and X_2 are the selfadjoint multiplication operators by the respective component of the position operator, i. e. $(X_i\psi)(\mathbf{x}) = x_i\psi(\mathbf{x})$, for $\psi \in \mathcal{D}(X_i)$.

Theorem 4.2.1 clearly holds true also for a projection admitting an exponentially localized GWB. Indeed, as we have underlined in Chapter 1, the exponential localization of the GWB implies that the basis is also s -localized for every $s > 0$.

We recall that for every operator A (possibly unbounded), the trace per unit volume \mathcal{T} that appears in equation (4.2.1) is defined by

$$\mathcal{T}(A) := \lim_{L \rightarrow +\infty} \frac{1}{|\Lambda_L|} \text{Tr}(\chi_{\Lambda_L} A \chi_{\Lambda_L})$$

where $\Lambda_L := [-L, L]^2 \subset \mathbb{R}^2$ and χ_{Λ_L} is the indicator function of the set Λ_L ¹. We say that the trace per unit volume of A exists whenever the right hand side exists and is finite.

¹Note that the function χ_{Λ_L} coincides with the previously defined function χ_L .

Before explaining the proof of Theorem 4.2.1 we show in the next section that the operator $\mathfrak{C}_L := \chi_{\Lambda_L} P_\mu [[X_1, P_\mu], [X_2, P_\mu]] \chi_{\Lambda_L}$ is a trace class operator, therefore equation (4.2.1) makes sense and can be rephrased in the following way. Suppose that the projection P_μ admits an s-localized GWB, then the function $\Xi : [0, +\infty) \rightarrow \mathbb{R}$ defined by

$$\Xi(L) := \frac{1}{|\Lambda_L|} \text{Tr}(\chi_{\Lambda_L} A \chi_{\Lambda_L}), \quad \forall L \in [0, +\infty)$$

is such that

$$\lim_{L \rightarrow +\infty} \Xi(L) = 0.$$

After that, in Section 4.4 we detail the proof of Theorem 4.2.1. We start by analysing the toy model case of compactly supported GWF. We use this simplified case as an example to explain the basic strategy of the general proof.

Remark 4.2.2. Notice that in the proof of Theorem 4.2.1 we will not use the “not too sparse” property of the Delone set. On the contrary, the “not too dense” property will be used in the proof of Proposition 4.3.2, which is crucial in the proof of Theorem 4.2.1. Despite of this fact, we decided to define the generalized Wannier basis, see Definition 1.3.6, in terms of Delone set since we believe that this mathematical object is the right generalization of a regular lattice. Future analysis on this issue is planned for the future.

Remark 4.2.3. As by-product of Theorem 4.2.1, we have that the dichotomic behaviour of the Wannier basis, summarized in Theorem 1.2.18, is “stable” with respect to regular perturbations. Indeed, fix a periodic system such that its Chern number is different from zero and suppose that we perturb the system with some small disordered potential like in Theorem 1.4.1. We want to show that the localization of the GWB cannot improve by perturbing the system with some regular (Kato small) perturbation. By contradiction, suppose that the perturbed system has an exponentially localized generalized Wannier basis. Applying Theorem 1.4.1, it is possible to unitarily transport the GWB back to the original system. Then, Theorem 4.2.1 implies that the Chern character is zero. Since we know from the results of Chapter 2 that the Chern character coincides with the Chern number in the case of periodic systems, we obtain a contradiction.

4.3 Well posedness of the problem

In this section we prove that the formal equation (4.2.1) has a precise mathematical meaning.

First of all, it is useful to rewrite (4.2.1) in terms of commutators of the so called *band position operators*. Let $\tilde{X}_j := P_\mu X_j P_\mu$ be the band position operator in direction $j \in \{1, 2\}$. Then by a direct computation, exploiting only $P_\mu^2 = P_\mu$ and $[X_1, X_2] = 0$, we get

$$\begin{aligned} & \chi_{\Lambda_L} P_\mu [[X_1, P_\mu], [X_2, P_\mu]] \\ &= \chi_{\Lambda_L} P X_1 P X_2 P - \chi_{\Lambda_L} P X_2 P X_1 P = \chi_{\Lambda_L} [\tilde{X}_1, \tilde{X}_2]. \end{aligned}$$

Thus (4.2.1) becomes

$$\mathcal{T} \left(i \left[\tilde{X}_1, \tilde{X}_2 \right] \right) = \lim_{L \rightarrow +\infty} \frac{1}{4L^2} \operatorname{Tr} \left(\chi_{\Lambda_L} i \left[\tilde{X}_1, \tilde{X}_2 \right] \chi_{\Lambda_L} \right). \quad (4.3.1)$$

Now we have to check that for all L , the operator $\chi_{\Lambda_L} \left[\tilde{X}_1, \tilde{X}_2 \right] \chi_{\Lambda_L}$ is trace class. Indeed, each term in the commutator is trace class thanks to the following proposition.

Proposition 4.3.1. *Consider the operators P_μ , X_i , $i = 1, 2$ and χ_{Λ_L} defined above. Then, for every $m, n \in \mathbb{N}$ the operator*

$$\chi_{\Lambda_L} P_\mu (X_i)^m P_\mu (X_j)^n$$

is a trace class operator.

Proof. Consider the β of estimate (1.3.7), let $3\eta < \beta$ and consider the multiplication operators $e^{-\eta\|X\|}$ and $e^{\eta\|X\|}$, then we have

$$\begin{aligned} & \chi_{\Lambda_L} P_\mu (X_i)^m P_\mu (X_j)^n \\ &= \chi_{\Lambda_L} e^{4\eta\|X\|} e^{-4\eta\|X\|} P_\mu e^{2\eta\|X\|} (X_i)^m e^{-2\eta\|X\|} P_\mu (X_j)^n. \end{aligned}$$

In view of the estimates (1.3.7) and the triangle inequality, we have that

$$\begin{aligned} & \left| \left(e^{-4\eta\|X\|} P_\mu e^{2\eta\|X\|} (X_i)^m \right) (\mathbf{x}; \mathbf{y}) \right| \leq C e^{-\eta\|\mathbf{x}\|} e^{-(\beta-3\eta)\|\mathbf{x}-\mathbf{y}\|}, \\ & \left| \left(e^{-2\eta\|X\|} P_\mu (X_j)^n \right) (\mathbf{x}; \mathbf{y}) \right| \leq C' e^{-(\beta-\eta)\|\mathbf{x}-\mathbf{y}\|} e^{-\eta\|\mathbf{x}\|}. \end{aligned}$$

Thus, the integral kernels of the two operators above are in $L^2(\mathbb{R}^2 \times \mathbb{R}^2)$ and hence they are Hilbert–Schmidt operators. Since the product of two Hilbert–Schmidt operators is in the trace class ideal, and $\chi_{\Lambda_L} e^{4\eta\|X\|}$ is a bounded operator, the proof is concluded. \square

Proposition 4.3.1 shows that the operator $\left[\tilde{X}_1, \tilde{X}_2 \right] \chi_{\Lambda_L}$ is a trace class operator, and since χ_{Λ_L} is a bounded operator, $\chi_{\Lambda_L} \left[\tilde{X}_1, \tilde{X}_2 \right] \chi_{\Lambda_L}$ is also trace class, hence equation (4.3.1) makes sense whenever the limit exists.

The mathematical core of the proofs is based on the estimates of discrete series evaluated on points of the Delone set \mathfrak{D} . Because of that, it is useful to have an easy way to estimate the value of the series we are interested in. The next proposition serves exactly this purpose.

Proposition 4.3.2. *Consider a continuous function*

$$D : \mathbb{R}^2 \rightarrow \mathbb{R},$$

such that $|D(\mathbf{x})| \geq |D(\mathbf{y})|$ whenever $|\mathbf{x}| \leq |\mathbf{y}|$. Then, there exists a constant K , independent of L , such that for every $L \gg 1$ it holds that

$$\sum_{\gamma \in \mathfrak{D} \cap \Lambda_{L,a}} |D(\gamma)| \leq K \int_{\Lambda_L} d\mathbf{x} |D(\mathbf{x})|. \quad (4.3.2)$$

Proof. The proof is based on the same argument of the well-known Maclaurin-Cauchy integral test. First of all, by definition of Delone set, we can find an r such that

$$\mathfrak{D} \cap B_r(\gamma) = \gamma, \quad \forall \gamma \in \mathfrak{D},$$

where $B_r(\gamma)$ is the open ball of radius r centred in γ . Consider now $\rho > r$ and all the points in \mathfrak{D} such that $|\gamma| \leq \rho$. By hypothesis on \mathfrak{D} , the number of points such that $|\gamma| < \rho$ is finite, so their contributions to the series is simply a constant, we call it K_ρ . Therefore we have

$$\sum_{\gamma \in \mathfrak{D} \cap \Lambda_{L,a}} |D(\gamma)| = K_\rho + \sum_{\gamma \in \mathfrak{D} \cap \Lambda_{L,a}, |\gamma| \geq \rho} |D(\gamma)|.$$

For every point $\gamma \in \mathfrak{D} \cap \Lambda_L$, such that $|\gamma| \geq \rho$ one can construct a square $A_r(\gamma)$ of area $\frac{r^2}{2}$ such that one of the vertices of the square is γ and for all $\mathbf{x} \in A_r(\gamma)$ it holds that $|\mathbf{x}| < |\gamma|$. Note that $A_r(\gamma)$ is exactly the square of diagonal length equal to r constructed along the line passing through the origin and γ . It is also true that

$$A_r(\gamma) \cap \mathfrak{D} = \gamma, \quad A_r(\gamma) \subset \Lambda_L.$$

Therefore, we obtain that

$$\begin{aligned} \sum_{\gamma \in \mathfrak{D} \cap \Lambda_{L,a}, |\gamma| \geq \rho} |D(\gamma)| &= \frac{2}{r^2} \sum_{\gamma \in \mathfrak{D} \cap \Lambda_{L,a}, |\gamma| \geq \rho} |D(\gamma)| \frac{r^2}{2} \\ &\leq \frac{2}{r^2} \sum_{\gamma \in \mathfrak{D} \cap \Lambda_{L,a}, |\gamma| \geq \rho} \int_{A_r(\gamma)} d\mathbf{x} |D(\mathbf{x})| \leq \frac{2m^*}{r^2} \int_{\Lambda_L} d\mathbf{x} |D(\mathbf{x})|. \end{aligned}$$

Then,

$$\sum_{\gamma \in \mathfrak{D} \cap \Lambda_{L,a}} |D(\gamma)| \leq \left(\frac{r^2 K_\rho}{2m^*} \left(\int_{\Lambda_\rho} d\mathbf{x} |D(\mathbf{x})| \right)^{-1} + 1 \right) \frac{2m^*}{r^2} \int_{\Lambda_L} d\mathbf{x} |D(\mathbf{x})|.$$

therefore the proof is concluded. \square

Remark 4.3.3. Note that we will extensively use the result of Proposition 4.3.2 through this section without explicitly referring to it every time.

4.4 Proof of Theorem 4.2.1

Before proceeding with the proof of Theorem 4.2.1, we first analyse a toy model situation, namely the case of a generalized Wannier basis that is *extremely localized*. The heuristic picture behind the toy model is the case of Wannier functions that are ‘‘almost delta functions’’ centred at the points of the irregular lattice \mathfrak{D} . We make use of this simple example to show the spirit of the proof and to introduce the operators Γ_i that will be useful in the proof of the general case.

4.4.1 Extremely localized GWB

Suppose that the Fermi projection admits a GWB made of generalized Wannier functions extremely localized, *i. e.* the support $\text{supp}\psi_{\gamma,a}$ of every GWF is compact and disjoint from the supports of the other GWFs, namely:

$$\begin{aligned} \text{supp}\psi_{\gamma,a} &\subset K_\gamma, & K_\gamma &\in \mathbb{R}^2, \\ \text{supp}\psi_{\gamma,a} \cap \text{supp}\psi_{\eta,b} &= \emptyset, & \forall (\gamma, a) \neq (\eta, b) &\in \mathcal{M}. \end{aligned} \quad (4.4.1)$$

Moreover we set

$$\langle \psi_{\gamma,a}, X_i \psi_{\gamma,a} \rangle =: f_i(\gamma, a), \quad i = \{1, 2\}. \quad (4.4.2)$$

Then we can proceed by explicitly calculating the trace. Consider an orthonormal basis for P_μ^\perp , $\{\phi_j\}_{j \in \mathcal{J}}$, and consider the set $\mathcal{I} = \mathcal{M} \cup \mathcal{J}$. Then, as a basis for the Hilbert space we take

$$\{e_i\}_{i \in \mathcal{I}} = \{\psi_{\gamma,a}\}_{(\gamma,a) \in \mathcal{M}} \cup \{\phi_j\}_{j \in \mathcal{J}}.$$

By definition of trace we have

$$\text{Tr}(\chi_{\Lambda_L} \tilde{X}_1 \tilde{X}_2 \chi_{\Lambda_L}) = \text{Tr}(\chi_{\Lambda_L} \tilde{X}_1 \tilde{X}_2) = \sum_i \langle e_i | \chi_{\Lambda_L} P_\mu X_1 P_\mu X_2 P_\mu | e_i \rangle \quad (4.4.3)$$

where in the first equality we used Proposition 4.3.1. Notice that

$$\begin{aligned} &\sum_i \sum_{\gamma,a} \sum_{\eta,b} \sum_{\xi,c} \langle e_i | \chi_{\Lambda_L} | \psi_{\gamma,a} \rangle \langle \psi_{\gamma,a} | X_1 | \psi_{\eta,b} \rangle \langle \psi_{\eta,b} | X_2 | \psi_{\xi,c} \rangle \langle \psi_{\xi,c} | e_i \rangle \\ &= \sum_{\gamma,a} \sum_{\eta,b} \sum_{\xi,c} \langle \psi_{\xi,c} | \chi_{\Lambda_L} | \psi_{\gamma,a} \rangle \langle \psi_{\gamma,a} | X_1 | \psi_{\eta,b} \rangle \langle \psi_{\eta,b} | X_2 | \psi_{\xi,c} \rangle. \end{aligned}$$

Consider now the terms $\langle \psi_{\gamma,a} | X_i | \psi_{\eta,b} \rangle$ with $i = 1, 2$. Since the X_i is a multiplication operator we have that $\text{supp}(X_i \psi_{\gamma,a}) \subseteq \text{supp}(\psi_{\gamma,a})$. Therefore, by the extremely localized hypothesis (4.4.1) and (4.4.2), we get

$$\begin{aligned} &\sum_{\gamma,a} \sum_{\eta,b} \sum_{\xi,c} \langle \psi_{\xi,c} | \chi_{\Lambda_L} | \psi_{\gamma,a} \rangle \langle \psi_{\gamma,a} | X_1 | \psi_{\eta,b} \rangle \langle \psi_{\eta,b} | X_2 | \psi_{\xi,c} \rangle \\ &= \sum_{\gamma,a} \sum_{\eta,b} \sum_{\xi,c} \langle \psi_{\xi,c} | \chi_{\Lambda_L} | \psi_{\gamma,a} \rangle \delta_{\gamma,\eta} \delta_{a,b} f_1(\gamma, a) \delta_{\eta,\xi} \delta_{b,c} f_2(\xi, b) \\ &= \sum_{\gamma,a} \langle \psi_{\gamma,a} | \chi_{\Lambda_L} | \psi_{\gamma,a} \rangle f_1(\gamma, a) f_2(\gamma, a). \end{aligned} \quad (4.4.4)$$

Note that the last sum involves only a finite number of GWFs, namely the ones such that $\text{supp}(\psi_{\gamma,a}) \cap \chi_{\Lambda_L} \neq 0$. Repeating the entire calculation for $\text{Tr}(\chi_{\Lambda_L} \tilde{X}_2 \tilde{X}_1)$ and using the linearity of the trace we obtain

$$\begin{aligned} &\text{Tr} \left(\chi_{\Lambda_L} \left(\tilde{X}_1 \tilde{X}_2 - \tilde{X}_2 \tilde{X}_1 \right) \right) \\ &= \sum_{\gamma,a} \langle \psi_{\gamma,a} | \chi_{\Lambda_L} | \psi_{\gamma,a} \rangle (f_1(\gamma, a) f_2(\gamma, a) - f_2(\gamma, a) f_1(\gamma, a)) = 0. \end{aligned} \quad (4.4.5)$$

Hence it is clear that also the limit for $L \rightarrow +\infty$ exists and it is equal to zero.

Thus, if the generalized Wannier functions are extremely localized, equation (4.2.1) holds true. Let us analyze the operators \tilde{X}_i in the case of an extremely localized generalized Wannier basis. From the definition of GWB we get that

$$\tilde{X}_i = \sum_{\gamma,a} \sum_{\eta,b} |\psi_{\gamma,a}\rangle \langle \psi_{\gamma,a}| X_i |\psi_{\eta,b}\rangle \langle \psi_{\eta,b}| = \sum_{\gamma,a} \gamma_i |\psi_{\gamma,a}\rangle \langle \psi_{\gamma,a}|.$$

This means that the unbounded operator \tilde{X}_i is a diagonal operator in the generalized Wannier basis representation, with eigenvalues given by the i -th coordinates of the points of \mathfrak{D} .

4.4.2 The operators Γ_i

Consider a GWB, with a generic localization function G (see Definition 1.3.6). In this case one cannot expect the operator \tilde{X}_i to be diagonal. Indeed, the expectation value of the position operators in the GWB, namely

$$\langle \psi_{\gamma,a}, X_i \psi_{\eta,b} \rangle,$$

could have non vanishing off-diagonal elements.

Therefore, we introduce the operators Γ_i ($i \in \{1, 2\}$) by

$$\Gamma_i := \sum_{\gamma,a} \gamma_i |\psi_{\gamma,a}\rangle \langle \psi_{\gamma,a}|, \quad (4.4.6)$$

which are defined on their maximal domains $\mathcal{D}(\Gamma_i)$. These operators will turn out to be useful for the further analysis. Let us now prove some interesting properties of the operators Γ_i .

Lemma 4.4.1. *The operators Γ_i defined in equation (4.4.6) are integral operators. Moreover*

- if $G(\|\mathbf{x}\|) = e^{2\alpha\|\mathbf{x}\|}$ the integral kernel $\Gamma_i(\mathbf{x}; \mathbf{y})$ satisfies

$$|\Gamma_i(\mathbf{x}; \mathbf{y})| \leq C e^{-\beta'\|\mathbf{x}-\mathbf{y}\|} + C' |x_i| e^{-\beta'\|\mathbf{x}-\mathbf{y}\|}$$

for $C, C' > 0$ and $\beta' < \alpha$.

- if $G(\|\mathbf{x}\|) = \langle \mathbf{x} \rangle^{2s}$, with $s > \frac{3}{2}$, the integral kernel $\Gamma_i(\mathbf{x}; \mathbf{y})$ satisfies

$$|\Gamma_i(\mathbf{x}; \mathbf{y})| \leq C \langle \mathbf{x} - \mathbf{y} \rangle^{-(s-\frac{3}{2}-\epsilon)} + C' |x_i| \langle \mathbf{x} - \mathbf{y} \rangle^{-(s-1-\epsilon)}$$

for every $\epsilon < s - \frac{3}{2}$.

Proof. Consider the case $G(\|\mathbf{x}\|) = e^{2\alpha\|\mathbf{x}\|}$. Then the formal integral kernel of Γ_i is given by

$$\Gamma_i(\mathbf{x}; \mathbf{y}) = \sum_{\gamma,a} \gamma_i \psi_{\gamma,a}(\mathbf{x}) \overline{\psi_{\gamma,a}(\mathbf{y})}.$$

For every fixed $\mathbf{x}, \mathbf{y} \in \mathbb{R}^2$ the sum over the indices $\{\gamma, a\}$ is absolutely convergent, namely

$$\begin{aligned} |\Gamma_i(\mathbf{x}; \mathbf{y})| &\leq \sum_{\gamma,a} \|\gamma - \mathbf{x}\| e^{-\alpha\|\mathbf{x}-\gamma\|} e^{-\alpha\|\mathbf{y}-\gamma\|} + \sum_{\gamma,a} |x_i| e^{-\alpha\|\mathbf{x}-\gamma\|} e^{-\alpha\|\mathbf{y}-\gamma\|} \\ &\leq C e^{-\beta'\|\mathbf{x}-\mathbf{y}\|} + C' |x_i| e^{-\beta'\|\mathbf{x}-\mathbf{y}\|}, \end{aligned} \quad (4.4.7)$$

where in the first inequality we have used the L^∞ estimate on the generalized Wannier function (1.3.8), in the second inequality we have used the property (1.3.1) of the localization function G and in the last inequality we have used Cauchy-Schwarz inequality. Hence the operators Γ_i admit an unbounded integral kernel. Consider now $G(\|\mathbf{x}\|) = \langle \mathbf{x} \rangle^{2s}$, with $s > \frac{3}{2}$. Since

$$\|x_i - \gamma\| \langle \mathbf{x} - \gamma \rangle^{-1} \leq C$$

for some positive constant C , we obtain

$$\begin{aligned} |\Gamma_i(\mathbf{x}; \mathbf{y})| &\leq \sum_{\gamma, a} \langle \mathbf{x} - \gamma \rangle^{-(s-1)} \langle \mathbf{y} - \gamma \rangle^{-s} + \sum_{\gamma, a} |x_i| \langle \mathbf{x} - \gamma \rangle^{-s} \langle \mathbf{y} - \gamma \rangle^{-s} \\ &\leq C_s \langle \mathbf{x} - \mathbf{y} \rangle^{-(s-\frac{3}{2}-\epsilon)} \sum_{\gamma, a} \langle \mathbf{y} - \gamma \rangle^{-(\frac{3}{2}+\epsilon)} \langle \mathbf{x} - \gamma \rangle^{-(\frac{1}{2}+\epsilon)} \\ &\quad + C_s |x_i| \langle \mathbf{x} - \mathbf{y} \rangle^{-(s-1-\epsilon)} \sum_{\gamma, a} \langle \mathbf{y} - \gamma \rangle^{-(1+\epsilon)} \langle \mathbf{x} - \gamma \rangle^{-(1+\epsilon)} \\ &\leq C \langle \mathbf{x} - \mathbf{y} \rangle^{-(s-\frac{3}{2}-\epsilon)} + C' |x_i| \langle \mathbf{x} - \mathbf{y} \rangle^{-(s-1-\epsilon)}, \end{aligned} \tag{4.4.8}$$

where again in the first inequality we have used L^∞ estimate on the GWF (1.3.8), in the second inequality we have used the property (1.3.1) of the localization function G and in the last inequality we have used Hölder's inequality. \square

Moreover, in view of the estimates on the integral kernels, the operators Γ_i obey some interesting trace class properties.

Proposition 4.4.2. *Consider the operators P_μ , X_i , Γ_i , for $i \in \{1, 2\}$ and χ_{Λ_L} defined above. Assume that the localization function is of polynomial type, with $s > \frac{9}{2}$, or exponentially growing. Then, for every $i, j \in \{1, 2\}$, $m, n \in \{0, 1\}$ the operator*

$$\chi_{\Lambda_L} P_\mu (X_i)^{1-m} \Gamma_i^m P_\mu (X_j)^{1-n} \Gamma_j^n,$$

is trace class.

Proof. The strategy of the proof is the same of Proposition 4.3.1. Let us show the computations explicitly for the case $i = 1, j = 2, m = 1, n = 0$ and $G(\|\mathbf{x}\|) = \langle \mathbf{x} \rangle^{2s}$.

We have that

$$\begin{aligned} &\chi_{\Lambda_L} P_\mu \Gamma_1 P_\mu X_2 \\ &= \chi_{\Lambda_L} e^{2\alpha\|X\|} e^{-2\alpha\|X\|} P_\mu e^{\alpha\|X\|} e^{-\alpha\|X\|} \Gamma_1 \langle X \rangle^{2+\epsilon} \langle X \rangle^{-2-\epsilon} P_\mu \langle X \rangle \langle X \rangle^{-1} X_2, \end{aligned}$$

for some $0 < \epsilon < 1$. Then, in view of estimate (1.3.7) and property (1.3.1) we have that

$$\left| \left(\langle X \rangle^{-2-\epsilon} P_\mu \langle X \rangle \right) (\mathbf{x}; \mathbf{y}) \right| \leq C \langle \mathbf{x} \rangle^{-2-\epsilon} e^{-\tilde{\beta}\|\mathbf{x}-\mathbf{y}\|}$$

for some positive constants $\tilde{\beta}, C$. Therefore $(\langle X \rangle^{-2-\epsilon} P_\mu \langle X \rangle)$ is a Hilbert–Schmidt operator. Similarly, considering (4.4.8) instead of (1.3.7), we have

$$\left| \left(e^{-\alpha\|X\|} \Gamma_1 \langle X \rangle^{2+\epsilon} \right) (\mathbf{x}; \mathbf{y}) \right| \leq e^{-\tilde{\alpha}\|\mathbf{x}\|} C \langle \mathbf{x} - \mathbf{y} \rangle^{-(s-\frac{7}{2}-2\epsilon)}.$$

where $0 < \tilde{\alpha} < \alpha$. Since $s > \frac{9}{2}$ the integral kernel of $(e^{-\alpha\|X\|} \Gamma_1 \langle X \rangle^{2+\epsilon})$ is in $L^2(\mathbb{R}^2 \times \mathbb{R}^2)$ and hence the operator is Hilbert–Schmidt. Moreover, $\langle X \rangle^{-1} X_2$ and $\chi_{\Lambda_L} e^{2\alpha\|X\|}$ are bounded operators and from the same computation in Proposition 4.3.1 we deduce that $(e^{-2\alpha\|X\|} P_\mu e^{\alpha\|X\|})$ is a bounded operator as well. This concludes the proof. \square

Remark 4.4.3. Although the proofs of Proposition 4.3.1 and Proposition 4.4.2 are very similar, their hypothesis have a fundamental difference. Proposition 4.3.1 requires only the localization of the integral kernel of the projection which in turn is based only on the existence of the gap in the spectrum of H , while Proposition 4.4.2 is based on the assumption of a GWB for the projection and on the particular decay of the GWFs, namely on the localization function G .

Note that the hypothesis of orthonormality of the GWB implies that

$$\begin{aligned} \Gamma_i P_\mu &= P_\mu \Gamma_i = \Gamma_i, \\ \Gamma_i \Gamma_j &= \Gamma_j \Gamma_i, \end{aligned}$$

and obviously, one has

$$\text{Tr}(\chi_{\Lambda_L} (\Gamma_i \Gamma_j - \Gamma_j \Gamma_i) \chi_{\Lambda_L}) = 0.$$

Therefore

$$\mathcal{T}([\Gamma_i, \Gamma_j]) = 0.$$

As we have seen in the previous section, in case of an extremely localized GWB we have that

$$\Gamma_i = \tilde{X}_i \quad i \in \{1, 2\}.$$

Heuristically speaking, the operators Γ_i represent the reduced position operators built with an ideal very well localized GWB. The strategy of the proof is to study “how far” the commutator between the reduced position operators is with respect to the commutator between the operators \tilde{X}_i . For our purpose the notion of “distance” (even if it is not a well defined distance) is encoded in the trace per unit volume. Therefore we are interested in proving

$$\mathcal{T}([\tilde{X}_1, \tilde{X}_2] - [\Gamma_1, \Gamma_2]) = 0.$$

4.4.3 Proof of Theorem 4.2.1

Let us now prove the main theorem. To make the proof as clear as possible we proceed in the following way. We first recollect all the important estimates on the GWB that we need for the proof in Proposition 4.4.4.

Proposition 4.4.4. *Let the hypothesis of Theorem 4.2.1 be satisfied, then there exist two positive constants $\mathcal{I}_{MO}, \mathcal{I}_{MI}$ such that*

$$\sum_{\xi \in \Lambda_L, c} \left\| \chi_{\Lambda_L^c} \psi_{\xi, c} \right\| \leq \mathcal{I}_{MO} L, \quad (4.4.9)$$

$$\sum_{\xi \notin \Lambda_L, c} \left\| \chi_{\Lambda_L} \psi_{\xi, c} \right\| \leq \mathcal{I}_{MI} L, \quad (4.4.10)$$

where we have defined $\chi_{\Lambda_L^c} := 1 - \chi_{\Lambda_L}$. Moreover there exist a function $F : [0, +\infty) \rightarrow [0, +\infty)$ and three positive constants I_1, I_2, I_3 such that

$$\sum_a^{m(\gamma)} \sum_b^{m(\eta)} |\langle \psi_{\gamma, a} | (X_i - \gamma_i) | \psi_{\eta, b} \rangle| \leq F(\|\gamma - \eta\|), \quad i = \{1, 2\}, \quad (4.4.11)$$

and F satisfies the following integrability conditions

$$\int_{\mathbb{R}^2} d\mathbf{x} F(\|\mathbf{x}\|) =: I_1 < \infty, \quad (4.4.12)$$

$$\int_{\mathbb{R}^2} d\mathbf{x} F(\|\mathbf{x}\|)^2 =: I_2 < \infty, \quad (4.4.13)$$

$$\int_{\mathbb{R}^2} d\mathbf{x} F(\|\mathbf{x}\|) \|\mathbf{x}\| =: I_3 < \infty. \quad (4.4.14)$$

$$\lim_{L \rightarrow +\infty} \frac{\int_{\Lambda_L} d\mathbf{x} \int_{\mathbb{R}^2 \setminus \Lambda_L} d\mathbf{y} F^2(\|\mathbf{x} - \mathbf{y}\|)}{L^2} = 0. \quad (4.4.15)$$

The proof of Proposition 4.4.4 is based on the one hand on the analysis of the distributions of the L^2 norm of the generalized Wannier functions with respect to the squares Λ_L , and on the other hand on a precise estimation of the off-diagonal elements of the operators \tilde{X}_i . All the details of the proof can be found in Section 4.4.4.

We stress that the decomposition of the integral kernel of P_μ as sum of generalized Wannier functions is crucial in order to prove Proposition 4.4.4.

After some simple algebraic manipulation, we get

$$\begin{aligned} & \chi_{\Lambda_L} \left([\tilde{X}_1, \tilde{X}_2] - [\Gamma_1, \Gamma_2] \right) \\ &= \chi_{\Lambda_L} \left[(\tilde{X}_1 - \Gamma_1), (\tilde{X}_2 - \Gamma_2) \right] + \chi_{\Lambda_L} \left[(\tilde{X}_1 - \Gamma_1), \Gamma_2 \right] + \chi_{\Lambda_L} \left[\Gamma_1, (\tilde{X}_2 - \Gamma_2) \right] \\ &=: T_1 + T_2 + T_3. \end{aligned}$$

In the following we will prove that

$$\lim_{L \rightarrow \infty} \text{Tr}(\chi_{\Lambda_L} T_j) = 0, \quad j \in \{1, 2, 3\}. \quad (4.4.16)$$

Estimate of the trace

In order to calculate explicitly the trace in (4.4.16), we follow the strategy delineated in the extremely localized case. First of all note that

$$\begin{aligned} \chi_{\Lambda_L} T_1 &= \chi_{\Lambda_L} (\tilde{X}_1 - \Gamma_1) P_\mu (\tilde{X}_2 - \Gamma_2) P_\mu - \chi_{\Lambda_L} P_\mu (\tilde{X}_2 - \Gamma_2) P_\mu (\tilde{X}_1 - \Gamma_1) P_\mu, \\ \chi_{\Lambda_L} T_2 &= \chi_{\Lambda_L} (\tilde{X}_1 - \Gamma_1) P_\mu \Gamma_2 P_\mu - \chi_{\Lambda_L} P_\mu \Gamma_2 P_\mu (\tilde{X}_1 - \Gamma_1) P_\mu, \\ \chi_{\Lambda_L} T_3 &= \chi_{\Lambda_L} \Gamma_1 P_\mu (\tilde{X}_2 - \Gamma_2) P_\mu - \chi_{\Lambda_L} P_\mu (\tilde{X}_2 - \Gamma_2) P_\mu \Gamma_1 P_\mu; \end{aligned}$$

where all the summands involved in the three equations are trace class due to Proposition 4.4.2. Exploiting the fact that the GWB is an orthonormal basis, we obtain

$$\begin{aligned} \text{Tr}(\chi_{\Lambda_L} T_1) &= \sum_{\xi,c} \sum_{\gamma,a} \sum_{\eta,b} \left[\langle \psi_{\xi,c} | \chi_{\Lambda_L} | \psi_{\gamma,a} \rangle \langle \psi_{\gamma,a} | (X_1 - \gamma_1) | \psi_{\eta,b} \rangle \langle \psi_{\eta,b} | (X_2 - \eta_2) | \psi_{\xi,c} \rangle \right. \\ &\quad \left. - \langle \psi_{\xi,c} | \chi_{\Lambda_L} | \psi_{\gamma,a} \rangle \langle \psi_{\gamma,a} | (X_2 - \gamma_2) | \psi_{\eta,b} \rangle \langle \psi_{\eta,b} | (X_1 - \eta_1) | \psi_{\xi,c} \rangle \right], \\ \text{Tr}(\chi_{\Lambda_L} T_2) &= \sum_{\xi,c} \sum_{\gamma,a} \langle \psi_{\xi,c} | \chi_{\Lambda_L} | \psi_{\gamma,a} \rangle \langle \psi_{\gamma,a} | (X_1 - \gamma_1) | \psi_{\xi,c} \rangle (\xi_2 - \gamma_2), \\ \text{Tr}(\chi_{\Lambda_L} T_3) &= \sum_{\xi,c} \sum_{\gamma,a} \langle \psi_{\xi,c} | \chi_{\Lambda_L} | \psi_{\gamma,a} \rangle \langle \psi_{\gamma,a} | (X_2 - \gamma_2) | \psi_{\xi,c} \rangle (\gamma_1 - \xi_1). \end{aligned}$$

We start with the trace of $\chi_{\Lambda_L} T_2$.

$$\begin{aligned} &\left| \sum_{\xi,c} \sum_{\gamma,a} \langle \psi_{\xi,c} | \chi_{\Lambda_L} | \psi_{\gamma,a} \rangle \langle \psi_{\gamma,a} | (X_1 - \gamma_1) | \psi_{\xi,c} \rangle (\xi_2 - \gamma_2) \right| \\ &\leq \sum_{\xi \in \Lambda_L, c} \sum_{\gamma,a} \delta_{\gamma,\xi} \delta_{a,c} |\langle \psi_{\gamma,a} | (X_1 - \gamma_1) | \psi_{\xi,c} \rangle (\xi_2 - \gamma_2)| \\ &\quad + \sum_{\xi \in \Lambda_L, c} \sum_{\gamma,a} \left| \langle \chi_{\Lambda_L^c} \psi_{\xi,c} | \psi_{\gamma,a} \rangle \langle \psi_{\gamma,a} | (X_1 - \gamma_1) | \psi_{\xi,c} \rangle (\xi_2 - \gamma_2) \right| \\ &\quad + \sum_{\xi \notin \Lambda_L, c} \sum_{\gamma,a} |\langle \chi_{\Lambda_L} \psi_{\xi,c} | \psi_{\gamma,a} \rangle \langle \psi_{\gamma,a} | (X_1 - \gamma_1) | \psi_{\xi,c} \rangle (\xi_2 - \gamma_2)| \\ &= T_{21} + T_{22} + T_{23}. \end{aligned}$$

The first series T_{21} , is zero after the summation in γ . The series T_{22}

$$\begin{aligned} &\sum_{\xi \in \Lambda_L, c} \sum_{\gamma,a} \left| \langle \chi_{\Lambda_L^c} \psi_{\xi,c} | \psi_{\gamma,a} \rangle \langle \psi_{\gamma,a} | (X_1 - \gamma_1) | \psi_{\xi,c} \rangle (\xi_2 - \gamma_2) \right| \\ &\leq \sum_{\xi \in \Lambda_L, c} \sum_{\gamma,a} \|\chi_{\Lambda_L^c} \psi_{\xi,c}\| F(\|\gamma - \xi\|) \|\gamma - \xi\| \leq I_3 \mathcal{I}_{MO} L, \end{aligned}$$

where in the last inequality we have used (4.4.9) and (4.4.14).

Series T_{23}

$$\begin{aligned} &\sum_{\xi \notin \Lambda_L, c} \sum_{\gamma,a} |\langle \chi_{\Lambda_L} \psi_{\xi,c} | \psi_{\gamma,a} \rangle \langle \psi_{\gamma,a} | (X_1 - \gamma_1) | \psi_{\xi,c} \rangle (\xi_2 - \gamma_2)| \\ &\leq \sum_{\xi \notin \Lambda_L, c} \sum_{\gamma,a} \|\chi_{\Lambda_L} \psi_{\xi,c}\| F(\|\gamma - \xi\|) \|\gamma - \xi\| \leq I_3 \mathcal{I}_{MI} L, \end{aligned}$$

where in the last inequality we have used (4.4.10) and (4.4.14).

We have obtained an asymptotic for the trace of $\chi_{\Lambda_L} T_2$: it goes at most linearly in L as $L \rightarrow \infty$.

The term T_3 is analogous to T_2 , hence it goes also at most linearly in L as $L \rightarrow \infty$.

Now it remains to study T_1 .

$$\sum_{\xi,c} \sum_{\gamma,a} \sum_{\eta,b} \left[\langle \psi_{\xi,c} | \chi_{\Lambda_L} | \psi_{\gamma,a} \rangle \langle \psi_{\gamma,a} | (X_1 - \gamma_1) | \psi_{\eta,b} \rangle \langle \psi_{\eta,b} | (X_2 - \eta_2) | \psi_{\xi,c} \rangle \right.$$

$$\begin{aligned}
& - \langle \psi_{\xi,c} | \chi_{\Lambda_L} | \psi_{\gamma,a} \rangle \langle \psi_{\gamma,a} | (X_2 - \gamma_2) | \psi_{\eta,b} \rangle \langle \psi_{\eta,b} | (X_1 - \eta_1) | \psi_{\xi,c} \rangle \Big] \\
= & \sum_{\xi \in \Lambda_L, c} \sum_{\gamma, a} \sum_{\eta, b} \left[\left(\delta_{\gamma, \xi} \delta_{a,c} \langle \psi_{\gamma,a} | (X_1 - \gamma_1) | \psi_{\eta,b} \rangle \langle \psi_{\eta,b} | (X_2 - \eta_2) | \psi_{\xi,c} \rangle \right. \right. \\
& - \delta_{\gamma, \xi} \delta_{a,c} \langle \psi_{\gamma,a} | (X_2 - \gamma_2) | \psi_{\eta,b} \rangle \langle \psi_{\eta,b} | (X_1 - \eta_1) | \psi_{\xi,c} \rangle \Big) \\
& - \left(\langle \chi_{\Lambda_L} \psi_{\xi,c} | \psi_{\gamma,a} \rangle \langle \psi_{\gamma,a} | (X_1 - \gamma_1) | \psi_{\eta,b} \rangle \langle \psi_{\eta,b} | (X_2 - \eta_2) | \psi_{\xi,c} \rangle \right. \\
& \left. \left. - \langle \chi_{\Lambda_L} \psi_{\xi,c} | \psi_{\gamma,a} \rangle \langle \psi_{\gamma,a} | (X_2 - \gamma_2) | \psi_{\eta,b} \rangle \langle \psi_{\eta,b} | (X_1 - \eta_1) | \psi_{\xi,c} \rangle \right) \right] \\
+ & \sum_{\xi \notin \Lambda_L, c} \sum_{\gamma, a} \sum_{\eta, b} \left[\langle \chi_{\Lambda_L} \psi_{\xi,c} | \psi_{\gamma,a} \rangle \langle \psi_{\gamma,a} | (X_1 - \gamma_1) | \psi_{\eta,b} \rangle \langle \psi_{\eta,b} | (X_2 - \eta_2) | \psi_{\xi,c} \rangle \right. \\
& \left. - \langle \chi_{\Lambda_L} \psi_{\xi,c} | \psi_{\gamma,a} \rangle \langle \psi_{\gamma,a} | (X_2 - \gamma_2) | \psi_{\eta,b} \rangle \langle \psi_{\eta,b} | (X_1 - \eta_1) | \psi_{\xi,c} \rangle \right] \\
= & \sum_{\xi \in \Lambda_L, c} \sum_{\gamma, a} \sum_{\eta, b} (R_1(\gamma, \eta, \xi) - R_2(\gamma, \eta, \xi)) + \sum_{\xi \notin \Lambda_L, c} \sum_{\gamma, a} \sum_{\eta, b} R_3(\gamma, \eta, \xi).
\end{aligned}$$

Notice that, a posteriori, we are allowed to split the series since we are going to prove that the series R_1, R_2 and R_3 are absolutely convergent. The series R_3 can be easily estimated

$$\begin{aligned}
& \sum_{\xi \notin \Lambda_L, c} \sum_{\gamma, a} \sum_{\eta, b} \left| \langle \chi_{\Lambda_L} \psi_{\xi,c} | \psi_{\gamma,a} \rangle \langle \psi_{\gamma,a} | (X_1 - \gamma_1) | \psi_{\eta,b} \rangle \langle \psi_{\eta,b} | (X_2 - \eta_2) | \psi_{\xi,c} \rangle \right. \\
& \quad \left. - \langle \chi_{\Lambda_L} \psi_{\xi,c} | \psi_{\gamma,a} \rangle \langle \psi_{\gamma,a} | (X_2 - \gamma_2) | \psi_{\eta,b} \rangle \langle \psi_{\eta,b} | (X_1 - \eta_1) | \psi_{\xi,c} \rangle \right| \\
& \leq \sum_{\xi \notin \Lambda_L, c} \sum_{\gamma, a} \sum_{\eta, b} \|\chi_{\Lambda_L} \psi_{\xi,c}\| 2F(\|\gamma - \eta\|) F(\|\eta - \xi\|) \\
& \leq 2I_1^2 \mathcal{I}_{MIL},
\end{aligned}$$

where in the last inequality we have used (4.4.10) and (4.4.12).

Now we study the absolute convergence of the series R_1 and R_2 . This allows to separate the series and to exchange the order of summation. Let us start with the series R_1

$$\begin{aligned}
& \sum_{\xi \in \Lambda_L, c} \sum_{\eta, b} |\langle \psi_{\xi,c} | (X_1 - \xi_1) | \psi_{\eta,b} \rangle \langle \psi_{\eta,b} | (X_2 - \eta_2) | \psi_{\xi,c} \rangle| \\
& \quad + |\langle \psi_{\xi,c} | (X_2 - \xi_2) | \psi_{\eta,b} \rangle \langle \psi_{\eta,b} | (X_1 - \eta_1) | \psi_{\xi,c} \rangle| \\
& \leq \sum_{\xi \in \Lambda_L, c} \sum_{\eta, b} 2F(\|\xi - \eta\|)^2 \leq I_2 K L^2,
\end{aligned}$$

where in the last inequality we have used (4.4.13).

Then, the series R_2 :

$$\begin{aligned}
& \sum_{\xi \in \Lambda_{L,c}} \sum_{\gamma, a} \sum_{\eta, b} \left| \left\langle \chi_{\Lambda_L^\xi} \psi_{\xi, c} \middle| \psi_{\gamma, a} \right\rangle \left\langle \psi_{\gamma, a} \middle| (X_1 - \gamma_1) \right\rangle \left\langle \psi_{\eta, b} \right\rangle \left\langle \psi_{\eta, b} \middle| (X_2 - \eta_2) \right\rangle \left| \psi_{\xi, c} \right\rangle \right| \\
& \quad + \left| \left\langle \chi_{\Lambda_L^\xi} \psi_{\xi, c} \middle| \psi_{\gamma, a} \right\rangle \left\langle \psi_{\gamma, a} \middle| (X_2 - \gamma_2) \right\rangle \left\langle \psi_{\eta, b} \right\rangle \left\langle \psi_{\eta, b} \middle| (X_1 - \eta_1) \right\rangle \left| \psi_{\xi, c} \right\rangle \right| \\
& \leq \sum_{\xi \in \Lambda_{L,c}} \sum_{\gamma, a} \sum_{\eta, b} \|\chi_{\Lambda_L^\xi} \psi_{\xi, c}\| 2F(\|\gamma - \eta\|) F(\|\xi - \eta\|) \leq 2I_1^2 \mathcal{I}_{MO} L,
\end{aligned}$$

where in the last inequality we have used (4.4.9) and (4.4.12).

Since the series are absolutely convergent we can study them separately. Proving the absolute convergence of the series R_2 has also shown that it goes at most linearly in L as $L \rightarrow \infty$.

Therefore so far we have shown that all the terms but the series R_1 go at most linearly in L . Thus, we need now to study in detail the series R_1 , namely

$$\begin{aligned}
& \sum_{\gamma, a} \sum_{\eta, b} \sum_{\xi \in \Lambda_{L,c}} \delta_{\gamma, \xi} \delta_{a, c} \langle \psi_{\gamma, a} \middle| (X_1 - \gamma_1) \rangle \langle \psi_{\eta, b} \rangle \langle \psi_{\eta, b} \middle| (X_2 - \eta_2) \rangle \left| \psi_{\xi, c} \right\rangle \\
& \quad - \sum_{\gamma, a} \sum_{\eta, b} \sum_{\xi \in \Lambda_{L,c}} \delta_{\gamma, \xi} \delta_{a, c} \langle \psi_{\gamma, a} \middle| (X_2 - \gamma_2) \rangle \langle \psi_{\eta, b} \rangle \langle \psi_{\eta, b} \middle| (X_1 - \eta_1) \rangle \left| \psi_{\xi, c} \right\rangle \\
& = \sum_{\eta, b} \sum_{\xi \in \Lambda_{L,c}} \langle \psi_{\xi, c} \middle| (X_1 - \xi_1) \rangle \langle \psi_{\eta, b} \rangle \langle \psi_{\eta, b} \middle| (X_2 - \eta_2) \rangle \left| \psi_{\xi, c} \right\rangle \\
& \quad - \sum_{\eta, b} \sum_{\xi \in \Lambda_{L,c}} \langle \psi_{\xi, c} \middle| (X_2 - \xi_2) \rangle \langle \psi_{\eta, b} \rangle \langle \psi_{\eta, b} \middle| (X_1 - \eta_1) \rangle \left| \psi_{\xi, c} \right\rangle.
\end{aligned}$$

Note that we have freely exchanged the order of summation because, as we have proved before, the series are absolute convergent.

For simplicity of notation we define

$$D(\eta, \xi) := \langle \psi_{\xi, c} \middle| (X_1 - \xi_1) \rangle \langle \psi_{\eta, b} \rangle \langle \psi_{\eta, b} \middle| (X_2 - \eta_2) \rangle \left| \psi_{\xi, c} \right\rangle. \quad (4.4.17)$$

Exchanging η and ξ in the second series, we get

$$\begin{aligned}
& \sum_{\eta, b} \sum_{\xi \in \Lambda_{L,c}} D(\eta, \xi) - \sum_{\eta, b \in \Lambda_L} \sum_{\xi, c} D(\eta, \xi) \\
& = \sum_{\eta \in \mathcal{D} \setminus \Lambda_L, b} \sum_{\xi \in \Lambda_{L,c}} D(\eta, \xi) - \sum_{\eta, b \in \Lambda_L} \sum_{\xi \in \mathcal{D} \setminus \Lambda_L, c} D(\eta, \xi).
\end{aligned} \quad (4.4.18)$$

Final Estimate

For our purpose we just need to study the asymptotic of the absolute value of the series of R_1 , that is

$$\begin{aligned}
& \left| \sum_{\eta \in \mathcal{D} \setminus \Lambda_L, b} \sum_{\xi \in \Lambda_{L,c}} D(\eta, \xi) - \sum_{\eta, b \in \Lambda_L} \sum_{\xi \in \mathcal{D} \setminus \Lambda_L, c} D(\eta, \xi) \right| \\
& \leq \sum_{\eta \in \mathcal{D} \setminus \Lambda_L, b} \sum_{\xi \in \Lambda_{L,c}} |D(\eta, \xi)| + \sum_{\eta, b \in \Lambda_L} \sum_{\xi \in \mathcal{D} \setminus \Lambda_L, c} |D(\eta, \xi)|
\end{aligned}$$

$$\leq 2 \sum_{\eta \in \mathfrak{D} \setminus \Lambda_L} \sum_{b \xi \in \Lambda_L, c} F^2(\|\eta - \xi\|).$$

It is clear from the definition of $|F(\eta, \xi)|$ that $|F(\eta, \xi)| \notin \ell^1(\mathfrak{D} \times \mathfrak{D})$. Hence we cannot simply apply Lebesgue dominated convergence theorem in order to perform the limit $L \rightarrow \infty$. Therefore we need to explicitly estimate the series. Now note that

$$|D(\eta, \xi)| \leq F^2(\|\eta - \xi\|). \quad (4.4.19)$$

Therefore, from the proof of equation (4.4.15) in Proposition 4.4.4, it follows that

$$\sum_{\eta \in \mathfrak{D} \setminus \Lambda_L} \sum_{b \xi \in \Lambda_L, c} F^2(\|\eta - \xi\|) \leq kL \text{ as } L \rightarrow \infty, \quad (4.4.20)$$

for some positive constant k . This proves that the trace per unit volume (4.3.1) goes to zero and the proof is concluded.

4.4.4 Proof of Proposition 4.4.4

This section is devoted to the proof of Proposition 4.4.4. We assume the following.

Assumption 4.4.5. Assume that P_μ admits a GWB s -localized, that is

$$G(\|\mathbf{x}\|) = \langle \mathbf{x} \rangle^{2s} \quad (4.4.21)$$

for some $s \geq s^* > 5$.

Let us start with the proof of equations (4.4.9) and (4.4.10). Under Assumption 4.4.5, the GWFs are not generally compactly supported but they are “mainly” concentrated on their centres. The strategy is to separate the contribution of each GWF in two terms: one that comes from the *centre* and the other that comes from the *tails*.

Consider $\Lambda_L \subset \mathbb{R}^2$. Let the centre of $\psi_{\gamma,a}$ be in Λ_L . To estimate “how much of $\psi_{\gamma,a}$ ” is outside Λ_L we look at the following

$$\left\| \chi_{\Lambda_L} \psi_{\gamma,a} - \psi_{\gamma,a} \right\| = \left\| \chi_{\Lambda_L^c} \psi_{\gamma,a} \right\| \quad (4.4.22)$$

where $\chi_{\Lambda_L^c}$ is the characteristic function of the complementary set of Λ_L .

$$\begin{aligned} \left\| \chi_{\Lambda_L^c} \psi_{\gamma,a} \right\| &= \left(\int_{\mathbb{R}^2} \chi_{\Lambda_L^c}(\mathbf{x}) \langle \mathbf{x} - \gamma \rangle^{2s} \langle \mathbf{x} - \gamma \rangle^{-2s} |\psi_{\gamma,a}(\mathbf{x})|^2 d\mathbf{x} \right)^{\frac{1}{2}} \\ &\leq \left(\sup_{\mathbf{x} \in \mathbb{R}^2} [\chi_{\Lambda_L^c}(\mathbf{x}) \langle \mathbf{x} - \gamma \rangle^{-2s}] \int_{\mathbb{R}^2} \langle \mathbf{x} - \gamma \rangle^{2s} |\psi_{\gamma,a}(\mathbf{x})|^2 d\mathbf{x} \right)^{\frac{1}{2}} \\ &\leq M^{\frac{1}{2}} \max \left\{ \langle L - |\gamma_1| \rangle^{-2s}, \langle L - |\gamma_2| \rangle^{-2s} \right\} \\ &\leq M^{\frac{1}{2}} \left(\langle L - |\gamma_1| \rangle^{-2s} + \langle L - |\gamma_2| \rangle^{-2s} \right). \end{aligned} \quad (4.4.23)$$

Instead, if the centre γ is outside Λ_L we have that

$$\begin{aligned}
\left\| \chi_{\Lambda_L} \psi_{\gamma,a} \right\| &= \left(\int_{\mathbb{R}^2} \chi_{\Lambda_L}(\mathbf{x}) |\psi_{\gamma,a}(\mathbf{x})|^2 d\mathbf{x} \right)^{\frac{1}{2}} \\
&\leq \left(\sup_{\mathbf{x} \in \mathbb{R}^2} \left[\chi_{\Lambda_L}(\mathbf{x}) \langle \mathbf{x} - \gamma \rangle^{-2s} \right] \int_{\mathbb{R}^2} \langle \mathbf{x} - \gamma \rangle^{2s} |\psi_{\gamma,a}(\mathbf{x})|^2 d\mathbf{x} \right)^{\frac{1}{2}} \\
&\leq M^{\frac{1}{2}} \left(\langle |\gamma_1| - L \rangle^{-2s} \chi_{A_1}(\gamma) + \langle |\gamma_2| - L \rangle^{-2s} \chi_{A_2}(\gamma) \right) \\
&\quad + M^{\frac{1}{2}} \langle \sqrt{||\gamma_1| - L|^2 + ||\gamma_2| - L|^2} \rangle^{-2s} \chi_{A_3}(\gamma).
\end{aligned} \tag{4.4.24}$$

Where $A_1 := ([-\infty, -L] \cup [L, \infty]) \times [-L, L]$, $A_2 := [-L, L] \times ([-\infty, -L] \cup [L, \infty])$ and $A_3 := \Lambda_L^c \setminus (A_1 \cup A_2)$, and χ_{A_i} , with $i \in \{1, 2, 3\}$, is the characteristic function of the set A_i .

The proof of (4.4.9) and (4.4.10) then follows easily by explicit integration. Before showing the computations, we recall the definition of some useful functions. Let us start from the modified Euler beta function $\tilde{\beta}(p, q)$ that is defined as follows

$$\tilde{\beta}(p, q) := \frac{\beta(p, q)}{2} = \int_0^{+\infty} dt \frac{t^{2p-1}}{(1+t^2)^{p+q}},$$

with p, q positive numbers in order to assure integrability. Notice that $\beta(p, q)$ is the usual Euler beta function. We also define, for every positive $x \in \mathbb{R}$, the modified incomplete Euler beta function by

$$\tilde{\beta}(p, q, x) := \int_0^x dt \frac{t^{2p-1}}{(1+t^2)^{p+q}}.$$

Moreover we set

$$\tilde{\beta}_c(p, q, x) := \tilde{\beta}(p, q) - \tilde{\beta}(p, q, x) = \int_x^{+\infty} dt \frac{t^{2p-1}}{(1+t^2)^{p+q}},$$

it is clear that $\tilde{\beta}_c(p, q, x)$ goes to zero as x goes to infinity.

Consider now the series in (4.4.9) and the estimate (4.4.23). Then, we have

$$\begin{aligned}
&\sum_{\xi \in \Lambda_{L,c}} \left\| \chi_{\Lambda_L^c} \psi_{\xi,c} \right\| \\
&\leq \sum_{\xi \in \Lambda_{L,c}} M^{\frac{1}{2}} \left[\langle L - |\gamma_1| \rangle^{-2s} + \langle L - |\gamma_2| \rangle^{-2s} \right] \\
&\leq \int_{-L}^L dx_1 \int_{-L}^L dx_2 M^{\frac{1}{2}} \left[\langle L - |x_1| \rangle^{-2s} + \langle L - |x_2| \rangle^{-2s} \right] \\
&\leq M^{\frac{1}{2}} 8L \int_0^{+\infty} dt \frac{1}{(1+t^2)^s} = M^{\frac{1}{2}} 8\tilde{\beta} \left(\frac{1}{2}, s - \frac{1}{2} \right) =: \mathcal{I}_{MOS} L.
\end{aligned} \tag{4.4.25}$$

This proves (4.4.9). Then consider the series in (4.4.10) and the estimate (4.4.24),

we get

$$\begin{aligned}
\sum_{\xi \notin \Lambda_L, c} \|\chi_{\Lambda_L} \psi_{\xi, c}\| &\leq M^{\frac{1}{2}} \sum_{\xi \notin \Lambda_L, c} \langle |\xi_1| - L \rangle^{-2s} \chi_{A_1}(\xi) \\
&\quad + M^{\frac{1}{2}} \sum_{\xi \notin \Lambda_L, c} \langle |\xi_2| - L \rangle^{-2s} \chi_{A_2}(\xi) \\
&\quad + \sum_{\xi \notin \Lambda_L, c} M^{\frac{1}{2}} \langle \sqrt{|\xi_1 - L|^2 + |\xi_2 - L|^2} \rangle^{-2s} \chi_{A_3}(\xi) \\
&\leq M^{\frac{1}{2}} 2 \int_L^{+\infty} dx_1 \int_{-L}^L dx_2 \langle |x_1| - L \rangle^{-2s} \\
&\quad + M^{\frac{1}{2}} 2 \int_{-L}^L dx_1 \int_L^{+\infty} dx_2 \langle |x_2| - L \rangle^{-2s} \\
&\quad + M^{\frac{1}{2}} 4 \int_L^{+\infty} dx_1 \int_L^{+\infty} dx_2 \langle \sqrt{|x_1 - L|^2 + |x_2 - L|^2} \rangle^{-2s} \\
&\leq M^{\frac{1}{2}} 8L \tilde{\beta} \left(\frac{1}{2}, s - \frac{1}{2} \right) + M^{\frac{1}{2}} \int_0^{\frac{\pi}{2}} d\theta \int_0^{+\infty} d\rho \frac{\rho}{(1 + \rho^2)^s} \\
&= M^{\frac{1}{2}} \left(\tilde{\beta} \left(\frac{1}{2}, s - \frac{1}{2} \right) 8 + \tilde{\beta} (1, s - 1) \frac{\pi}{2L} \right) L \\
&< M^{\frac{1}{2}} \left(\tilde{\beta} \left(\frac{1}{2}, s - \frac{1}{2} \right) 8 + \tilde{\beta} (1, s - 1) \frac{\pi}{2} \right) L =: \mathcal{I}_{MIS} L.
\end{aligned} \tag{4.4.26}$$

Now it remains to prove the second part of Proposition 4.4.4, the one regarding the off-diagonal terms of \tilde{X}_i . Let us begin by proving the existence of the function F satisfying (4.4.11). In the extremely localized case we can take F to be any smooth function that is equal to 1 at the origin and it is fast decaying as $\mathbf{x} \rightarrow \infty$. Instead, in this case the decay at infinity will be determined by the localization function G . Consider the generic matrix element of $\tilde{X}_1 - \Gamma_1$, we have that

$$\begin{aligned}
&\sum_a^{m(\gamma)} \sum_b^{m(\eta)} |\langle \psi_{\gamma, a} | (X_1 - \gamma_1) | \psi_{\eta, b} \rangle| \\
&\leq (m^*)^2 \max_{a \leq m(\gamma)} \max_{b \leq m(\eta)} |\langle \psi_{\gamma, a} | (X_1 - \gamma_1) | \psi_{\eta, b} \rangle| \\
&\leq (m^*)^2 \int_{\mathbb{R}^2} d\mathbf{x} |\psi_{\gamma, \tilde{a}}(\mathbf{x})| |x_1 - \gamma_1| |\psi_{\eta, \tilde{b}}(\mathbf{x})|.
\end{aligned}$$

Where \tilde{a} and \tilde{b} are the maximizers of $|\langle \psi_{\gamma, a} | (X_1 - \gamma_1) | \psi_{\eta, b} \rangle|$. Taking into account the L^∞ estimate (1.3.8) we get that, for $\epsilon > 0$ small enough, it holds

$$\begin{aligned}
&(m^*)^2 \int_{\mathbb{R}^2} d\mathbf{x} |\psi_{\gamma, \tilde{a}}(\mathbf{x})| |x_1 - \gamma_1| |\psi_{\eta, \tilde{b}}(\mathbf{x})| \\
&\leq (m^*)^2 \int_{\mathbb{R}^2} d\mathbf{x} \langle \mathbf{x} - \gamma \rangle^{-s} |x_1 - \gamma_1| \langle \mathbf{x} - \eta \rangle^{-s} \\
&\leq (m^*)^2 \int_{\mathbb{R}^2} d\mathbf{x} \langle \mathbf{x} - \gamma \rangle^{-(s-2-\epsilon)} \langle \mathbf{x} - \eta \rangle^{-(s-2-\epsilon)} \langle \mathbf{x} - \eta \rangle^{-(2+\epsilon)} \\
&\leq C_s (m^*)^2 \langle \gamma - \eta \rangle^{-(s-2-\epsilon)},
\end{aligned}$$

where in the last inequality we used property (1.3.1) of the localization function and the translation invariance of the integral. The same computation goes through exchanging $X_1 - \gamma_1$ with $X_2 - \gamma_2$, therefore, we have that the function F defined by

$$F(\|\mathbf{x}\|) := C_s(m^*)^2 \langle \mathbf{x} \rangle^{-(s-2-\epsilon)}$$

satisfies (4.4.11). By direct simple computations, one can show that F satisfies also the requirements (4.4.12) for every $s > 4$, (4.4.13) for every $s > 3$ and (4.4.14) for every $s > 5$. This is the reason why the threshold in Theorem 4.2.1 is $s^* > 5$. The last requirement, (4.4.15), is a consequence of the next computation, which shows that (4.4.15) is satisfied for every $s > 7/2$. Indeed, consider the integral

$$\int_{\Lambda_L} d\mathbf{x} \int_{\mathbb{R}^2 \setminus \Lambda_L} d\mathbf{y} \frac{1}{(1 + \|\mathbf{x} - \mathbf{y}\|^2)^\alpha}. \quad (4.4.27)$$

Since the integrand is positive the order of integration does not affect the result. For a fixed $\mathbf{x} \in \Lambda_L$ we have the inequality

$$\frac{1}{(1 + \|\mathbf{x} - \mathbf{y}\|^2)^\alpha} \leq \frac{1}{(1 + \|\mathbf{x} - \mathbf{y}\|^2)^{\frac{\alpha}{2}}} \frac{1}{(1 + (\text{dist}(\mathbf{x}, \partial\Lambda_L))^2)^{\frac{\alpha}{2}}}.$$

By integrating with respect to \mathbf{y} we obtain

$$\begin{aligned} & \int_{\Lambda_L} d\mathbf{x} \int_{\mathbb{R}^2 \setminus \Lambda_L} d\mathbf{y} \frac{1}{(1 + \|\mathbf{x} - \mathbf{y}\|^2)^\alpha} \\ & \leq \int_{\Lambda_L} d\mathbf{x} \int_{\mathbb{R}^2 \setminus \Lambda_L} d\mathbf{y} \frac{1}{(1 + \|\mathbf{x} - \mathbf{y}\|^2)^{\frac{\alpha}{2}}} \frac{1}{(1 + (\text{dist}(\mathbf{x}, \partial\Lambda_L))^2)^{\frac{\alpha}{2}}} \\ & \leq 2\pi\tilde{\beta} \left(1, \frac{\alpha}{2} - 1\right) \int_{\Lambda_L} d\mathbf{x} (\text{dist}(\mathbf{x}, \partial\Lambda_L))^2)^{\frac{\alpha}{2}}, \end{aligned}$$

Notice that last inequality requires $\alpha > 2$. The integral with respect to \mathbf{x} can be now easily estimated by

$$\int_{\Lambda_L} d\mathbf{x} \frac{1}{(1 + (\text{dist}(\mathbf{x}, \partial\Lambda_L))^2)^{\frac{\alpha}{2}}} \leq 8\tilde{\beta} \left(1, \frac{\alpha}{2} - 1\right) + 8\tilde{\beta} \left(\frac{1}{2}, \frac{\alpha}{2} - \frac{1}{2}\right) L = \mathcal{O}(L),$$

where the last inequality requires $\alpha > 2$, which means that $s > 4$. This concludes the proof of Proposition 4.4.4.

Chapter 5

Parseval frames of exponentially localized magnetic Wannier functions

Exponentially localized Wannier basis for a given spectral projection are a very effective mathematical tool, however, as we recalled in Chapter 1, they do not always exist. In this chapter we show that, even though there are cases where the desirable exponentially localized Wannier basis is not constructible, it is always possible to construct a Parseval frame of exponentially localized Wannier-like functions. As a by-product of our proof, we show how to extend the proof “by continuity” of the existence of a generalized Wannier basis for systems that are not time-reversal symmetric. This chapter reproduces the content of the article [33], which is the fruit of a joint collaboration with H. Cornean and D. Monaco.¹

Specifically, motivated by the analysis of gapped periodic quantum systems in presence of a uniform magnetic field in dimension $d \leq 3$, we study the possibility to construct spanning sets of exponentially localized (generalized) Wannier functions for the space of occupied states.

When the magnetic flux per unit cell satisfies a certain rationality condition, by going to the momentum-space description one can model m occupied energy bands by a real-analytic and \mathbb{Z}^d -periodic family $\{P(\mathbf{k})\}_{\mathbf{k} \in \mathbb{R}^d}$ of orthogonal projections of rank m . A moving *orthonormal basis* of $\text{Ran } P(\mathbf{k})$ consisting of real-analytic and \mathbb{Z}^d -periodic Bloch vectors can be constructed if and only if the first Chern number(s) of P vanish(es). Here we are mainly interested in the topologically obstructed case.

First, by dropping the generating condition, we show how to algorithmically construct a collection of $m - 1$ *orthonormal*, real-analytic, and \mathbb{Z}^d -periodic Bloch vectors. Second, by dropping the linear independence condition, we construct a *Parseval frame* of $m + 1$ real-analytic and \mathbb{Z}^d -periodic Bloch vectors which generate $\text{Ran } P(\mathbf{k})$. Both algorithms are based on a two-step logarithm method which produces a moving orthonormal basis in the topologically trivial case.

¹In the current version of the thesis, Chapter 5 has been modified according to the version of the paper [33] that has been accepted for publication in *Communication in Mathematical Physics*. The mathematical results are the same but the exposition has been improved. The previous version can be found at the link <https://arxiv.org/abs/1704.00932v3>.

A moving Parseval frame of analytic, \mathbb{Z}^d -periodic Bloch vectors corresponds to a Parseval frame of exponentially localized composite Wannier functions. We extend this construction to the case of magnetic Hamiltonians with an irrational magnetic flux per unit cell and show how to produce Parseval frames of exponentially localized generalized Wannier functions also in this setting.

Our results are illustrated in crystalline insulators modelled by $2d$ discrete Hofstadter-like Hamiltonians, but apply to certain continuous models of magnetic Schrödinger operators as well.

5.1 Introduction

As we have extensively recalled in Chapter 1, a large number of problems coming from the condensed matter physics of crystalline insulators can be mathematically described by means of a gapped Hamilton operator, where the gap in the spectrum is a threshold for the occupied states. In this framework it is important to have a suitable set of vectors in the Hilbert space that represents this energy window and encodes all the relevant physical information contained in the gapped spectral island. The reasons for that are multiple: from a theoretical point of view, one needs, for example, to justify the use of effective Hamiltonians, say of tight-binding nature, that simplify the analysis of the model while retaining the relevant features of the underlying physical system; from the computational point of view, the use of a suitable basis allows the efficient computation of physical quantities [55, 116, 100, 108, 74].

Summarizing the discussion of Section 1.2, we have that when the gapped Hamiltonian is *periodic*, then it is possible to pass to the \mathbf{k} -space representation through the *Bloch–Floquet transform* [71], and the space of occupied states is described by a \mathbb{Z}^d -periodic family of projections $P(\mathbf{k})$, where $d \leq 3$ is the dimension of the system. The associated Bloch bundle [89, 77], the vector bundle over the Brillouin torus $\mathbb{T}^d := \mathbb{R}^d/\mathbb{Z}^d \simeq (-1/2, 1/2)^d$ whose fiber over \mathbf{k} is the space $\text{Ran } P(\mathbf{k}) \subset L^2((0, 1)^d)$ of occupied states at fixed crystal momentum \mathbf{k} , contains all the physical information pertaining the relevant gapped spectral island. A suitable set of vectors spanning this space consists then of sections $\{\xi_a(\mathbf{k})\}_{a \in \{1, \dots, M\}}$ of the Bloch bundle. The inverse Bloch–Floquet transform

$$w_a(\underline{x} + \gamma) := \int_{(-1/2, 1/2)^d} d\mathbf{k} e^{i2\pi\mathbf{k}\cdot\gamma} \xi_a(\mathbf{k}, \underline{x}), \quad \underline{x} \in (0, 1)^d, \gamma \in \mathbb{Z}^d, \quad (5.1.1)$$

defines then (*composite*) *Wannier functions*, which together with their translates span the gapped spectral island of the Hamiltonian. For the theoretical purposes mentioned above, it is important that these Wannier functions decay at infinity as fast as possible, e.g. exponentially: by a Paley–Wiener-type argument, this is equivalent to requiring that the Bloch vectors $\xi_a(\mathbf{k})$ depend analytically on \mathbf{k} [42, 41, 71].

The first goal of this chapter is to provide a *constructive algorithm* that produces such a spanning set of localized Wannier functions, or rather the corresponding Bloch vectors. Notice that in general the existence of an *orthormal basis* of (continuous, periodic) Bloch vectors is *topologically obstructed* by the geometry of the Bloch bundle [112, 111, 66, 89, 76] (see Section 5.3). However, if one relaxes the linear independence condition, then this topological obstruction can be circumvented

[3, 70, 71]: we provide a new proof of this result (formulated here as Theorem 5.3.2) in the form of an algorithm for the construction of a “redundant”, non-orthonormal spanning set of Bloch vectors (a *Parseval frame*, to be precise). As we will detail in Section 5.3.2, this datum is sufficient for example to recover spectral properties and construct effective models associated to the original Hamiltonian, even in lack of orthonormality and linear independence.

This first result, applies to both continuous and discrete models of 2- and 3-dimensional gapped crystals subject to a constant magnetic field whose flux per unit cell satisfies a certain commensurability condition. In this chapter, we choose as a recurring example the model of Hofstadter-like Hamiltonians, which are discrete analogues of magnetic Schrödinger operators on the 2-dimensional lattice \mathbb{Z}^2 with uniform magnetic field in the orthogonal direction. Hofstadter-like Hamiltonians will be described in detail in Section 5.2; the application of the general result Theorem 5.3.2 to these models is spelled out in Theorem 5.3.4.

When periodicity is lost, there is no underlying vector bundle structure for the occupied states, and so the quest for a suitable set of spanning vectors becomes more complicated. However, the question is still well-defined in the original position-space representation, and one can ask whether a spanning set of localized (generalized) Wannier functions exists.

To describe this non-periodic setting we specialize, for the sake of a more explicit presentation, to Hofstadter-like Hamiltonians. Up to an explicit unitary “scaling” transformation depending on the magnetic field (which corresponds roughly speaking to considering a supercell for the lattice), these Hamiltonians become periodic under the above-mentioned commensurability condition on the magnetic flux per unit cell, see Proposition 5.2.1. Very concretely, in our case this condition requires that the strength of the magnetic field be a rational multiple of 2π . For a value b_0 for which the latter condition is satisfied, we can apply the result from the first part, which yields a Parseval frame of localized Wannier functions for every gapped spectral island.

Perturbing around $b_0 \in 2\pi\mathbb{Q}$, say for $b = b_0 + \epsilon$ with $\epsilon \ll 1$, the spectral island remains gapped but periodicity is lost when $\epsilon/(2\pi)$ is irrational [87]. Nevertheless, if ϵ is small enough, we will show how one can *extend* the construction of a Parseval frame of localized generalized Wannier functions for the spectral island at magnetic field b_0 to one at magnetic field b , see Theorem 5.4.1 and its Corollary 5.4.3. The result essentially depends on Combes–Thomas exponential estimates for the resolvent of the Hamiltonian. Once again, all the results for the type of discrete magnetic Hamiltonians discussed above can be extended to continuous models and magnetic Schrödinger operators, see Remark 5.9.7.

5.1.1 Comparison with the literature

We would like here to compare our results with the existing literature on the subject.

The most novel contributions in this chapter are given by Theorem 5.4.1 and its Corollary 5.4.3 concerning the construction of spanning sets of localized Wannier functions for magnetic Hamiltonians with an *irrational* magnetic flux. These provide in particular a generalization in the discrete setting of the results of [30] which assume *time-reversal symmetry* (hence zero magnetic flux per unit cell), consequently

covering only the periodic case with no topological obstruction to the existence of an orthonormal basis of localized Wannier functions, and perturbations theorem.

The literature on the interplay between topology and existence of localized Wannier functions in gapped *periodic* quantum systems is much more extended. Concerning the topologically trivial case, namely when the existence of an orthonormal basis is not topologically obstructed, our proof of Theorem 5.3.2(iii) (correspondingly Theorem 5.3.4(ii)) provides a constructive algorithm for the results of [89, 77] (compare also [70]), which are instead obtained by abstract bundle-theoretic methods. There, the condition of topological triviality is obtained as a consequence of time-reversal symmetry: constructive algorithms for Bloch bases under this symmetry assumption have been recently investigated in [47, 46, 23, 30, 34, 31].

Moving to the topologically non-trivial setting, to the best of our knowledge the only previous work which treated the problem of constructing an effective magnetic Hamiltonian starting from a topologically obstructed Fermi projection is [49]. However, there the authors only allow bounded magnetic potentials as perturbations, thus excluding magnetic fields which do not vanish at infinity.

Even though the use of “non-orthogonal Wannier functions” (that is, of redundant spanning sets of Wannier functions) is adopted in several computational schemes for electronic structure, quantum chemistry and density functional theory [50, 55, 74], in the mathematical literature the study of Parseval (or equivalently 1-tight) frames of localized Wannier functions in the topologically obstructed case was initiated only in [70], where an upper bound of the form $M \leq 2^d m$ was given on the number of Bloch vectors needed to span m isolated energy bands in dimension d . Improved estimates on M for Bloch bundles in $d \leq 3$ were announced in [71] and proved in [3], yielding $M = m + 1$ as in Theorem 5.3.2(ii) (correspondingly Theorem 5.3.4(ii)). The results of [3] prove the *existence* of a Parseval $(m + 1)$ -frame of exponentially localized Wannier functions when $d \leq 3$, again by means of general bundle-theoretic arguments. However, using powerful results from the theory of functions of several complex variables, their proofs allow to show that the corresponding Bloch vectors are analytic in the *same analyticity domain* of the family of projections $\{P(\mathbf{k})\}_{\mathbf{k} \in \mathbb{R}^d}$. Our techniques, even though more algorithmic and “explicit” in nature, allow instead only to exhibit Bloch vectors which are *real-analytic*, that is, analytic in a complex strip around the real axis which could in principle be much smaller than the analyticity domain of the map $\mathbf{k} \mapsto P(\mathbf{k})$. The problem of finding an explicit extension of these Bloch vectors to this domain (again through “algorithmic” methods) is an interesting research line, which we postpone to future investigation.

In this respect, it is also interesting to notice that exponential localization of generalized Wannier Parseval frames is somewhat optimal. Indeed, it was recently proved in [43] that if one requires the Wannier functions in a Parseval frame to be *compactly supported*, then necessarily the Bloch bundle must be trivial.

5.1.2 Structure of the chapter

The chapter consists of three main parts.

The first part is devoted to the presentation of the reference physical model, namely Hofstadter-like Hamiltonians, in Section 5.2, and of our main contributions, whose proofs are postponed to the remaining two parts of the chapter, in Sections 5.3

and 5.4. In particular, in Section 5.3 we present Theorem 5.3.2 on spanning sets of vectors for periodic families of projections, as well as its application to Hofstadter-like Hamiltonians with rational magnetic flux, that is, Theorem 5.3.4. After that, in Section 5.4 we describe the extension of these results to Hofstadter-like Hamiltonians with irrational but close-to-rational magnetic flux, namely Theorem 5.4.1 and its Corollary 5.4.3. A brief outline of the constructive, algorithmic proof for these results can be found in the discussion after Corollary 5.4.3.

The second part of the chapter focuses on our new proof of Theorem 5.3.2, which is spread through Sections 5.5 to 5.7: in Section 5.5 we prove the third part of Theorem 5.3.2 regarding the periodic topologically trivial case, in Section 5.6 we prove the first part of Theorem 5.3.2 on the maximal number of orthonormal vectors, and finally in Section 5.7 we construct the Parseval frame for projections with non-trivial topology. In the context of Hofstadter-like Hamiltonians, by going back to position-space via the inverse Bloch–Floquet transform (5.1.1) this will prove also Theorem 5.3.4.

The last part of the chapter is instead concerned with the proofs of Theorem 5.4.1 and Corollary 5.4.3. In Section 5.8 we show that the problem of finding Parseval frames of localized Wannier functions for general Hofstadter-like Hamiltonians can be recast in a more abstract problem regarding Fermi-like magnetic projections, see Definition 5.8.2 and Lemma 5.8.4. In the last Section 5.9 we construct the required Parseval frame and conclude the proof of Theorem 5.4.1.

5.2 The reference model: Hofstadter-like Hamiltonians

This section presents our motivating physical model of crystalline systems in presence of uniform magnetic fields; we fix here some notation that will be used extensively throughout the chapter. The quantum systems of interest are modelled by magnetic Hamiltonians, like e.g. discrete tight-binding Hamiltonians where hoppings carry Peierls magnetic phases, or continuous Schrödinger operators of the form $\frac{1}{2}(-i\nabla - A)^2 + V$, where A (respectively V) is the magnetic (respectively electrostatic) potential. To fix a reference model, to be used in applications of more general results, we now introduce Hofstadter-like Hamiltonians in the 2-dimensional discrete setting.

Consider a set of N points $\mathcal{Y} \subset [0, 1]^2 \subset \mathbb{R}^2$, and a collection of functions $h_{\mathbf{k}}: \mathcal{Y} \times \mathcal{Y} \rightarrow \mathbb{R}$ which are real-analytic and \mathbb{Z}^2 -periodic in \mathbf{k} , meaning that the maps $\mathbb{R}^2 \ni \mathbf{k} \mapsto h_{\mathbf{k}}(\underline{y}, \underline{y}') \in \mathbb{R}$ with fixed $\underline{y}, \underline{y}' \in \mathcal{Y}$ are real-analytic and \mathbb{Z}^2 -periodic. Let us also introduce the skew-symmetric Peierls magnetic phase $\phi: \mathbb{R}^2 \times \mathbb{R}^2 \rightarrow \mathbb{R}$, defined by

$$\phi(\mathbf{x}, \mathbf{x}') := (x'_1 x_2 - x'_2 x_1)/2 = \{\mathbf{e}_3 \cdot (\mathbf{x}' \times \mathbf{x})\}/2. \quad (5.2.1)$$

We define, for $b \in \mathbb{R}$, the bounded operator in $\ell^2(\mathbb{Z}^2 \times \mathcal{Y}) \simeq \ell^2(\mathbb{Z}^2) \otimes \ell^2(\mathcal{Y})$ (note that $\ell^2(\mathcal{Y}) \simeq \mathbb{C}^N$) given by the following matrix elements:

$$\begin{aligned} H_b(\gamma, \underline{y}; \gamma', \underline{y}') &:= e^{ib\phi(\gamma+\underline{y}, \gamma'+\underline{y}')} \mathcal{T}(\gamma - \gamma'; \underline{y}, \underline{y}'), \\ \text{where } \mathcal{T}(\gamma; \underline{y}, \underline{y}') &:= \int_{\Omega} d\mathbf{k} e^{i2\pi\mathbf{k}\cdot\gamma} h_{\mathbf{k}}(\underline{y}, \underline{y}') \end{aligned} \quad (5.2.2)$$

with $\gamma, \gamma' \in \mathbb{Z}^2$, $\underline{y}, \underline{y}' \in \mathcal{Y}$, and the integral defining \mathcal{T} is performed over $\Omega := (-1/2, 1/2)^2$. Then $h_{\mathbf{k}}$ can be recovered via

$$h_{\mathbf{k}}(\underline{y}, \underline{y}') = \sum_{\gamma \in \mathbb{Z}^2} e^{-i2\pi \mathbf{k} \cdot \gamma} \mathcal{T}(\gamma; \underline{y}, \underline{y}'), \quad \underline{y}, \underline{y}' \in \mathcal{Y}, \mathbf{k} \in \mathbb{R}^2.$$

The resulting operator H_b will be called an *Hofstadter-like Hamiltonian*; the original Hofstadter model [62] would correspond to $\mathcal{Y} = \{(0, 0)\}$ (i.e. $N = 1$), $h_{\mathbf{k}} = 2 \cos(2\pi k_1) + 2 \cos(2\pi k_2)$, while the Peierls phase would be written in the Landau gauge and equal $\phi_L(\mathbf{x}, \mathbf{x}') := (x_2 - x_2')(x_1 + x_1')/2$. The magnetic phase $e^{ib\phi(\cdot, \cdot)}$ in front of the “hopping” \mathcal{T} models the presence of a uniform magnetic field $\mathbf{B} := b \mathbf{e}_3$ orthogonal to the 2-dimensional crystal. The quantity $-2b\phi(\mathbf{e}_1, \mathbf{e}_2) = \mathbf{B} \cdot (\mathbf{e}_1 \times \mathbf{e}_2)$ is then the magnetic flux per unit cell, to be measured in units of the magnetic flux quantum (which equals $1/2\pi$ in our units).

When $b = 0$ the spectrum of H_0 is absolutely continuous and it is given by the range of the N eigenvalues $E_j(\mathbf{k})$ of $h_{\mathbf{k}}$ as functions of \mathbf{k} , that is,

$$\sigma(H_0) = \{E \in \mathbb{R} : E_j(\mathbf{k}) = E \text{ for some } j \in \{1, \dots, N\}, \mathbf{k} \in \Omega\}.$$

The graph of the function E_j is usually called the j -th energy (Bloch) band. Several analytic properties of these non-magnetic energy bands are discussed in [5], see also [118] for the infinite-dimensional generalization from \mathbf{k} -dependent matrices to linear operators on Banach spaces.

If the magnetic field strength b is such that $b = b_0$ where $b_0/(2\pi)$ is rational, i.e. there exists $q \in \mathbb{N}$ such that $b_0 q \in 2\pi\mathbb{Z}$, then H_{b_0} is unitarily equivalent to a periodic operator. Notice that the condition $b_0 \in 2\pi\mathbb{Q}$ implies that the magnetic flux per unit cell is a rational multiple of the flux quantum: we will thus call this the “rational flux” condition. In order to formulate this unitary equivalence more precisely, and to be able to study also values of the magnetic field strength b which are close to b_0 , we will use the common technique of enlarging the unit cell in order to have an integer-flux magnetic field: we introduce the new lattice $\Gamma_q := (q\mathbb{Z}) \times \mathbb{Z} \simeq \mathbb{Z}^2$ and denote by \mathcal{Y}_q its fundamental cell, namely

$$\mathcal{Y}_q = \mathcal{B}_q \times \mathcal{Y} \subset \mathbb{R}^2, \quad \text{where } \mathcal{B}_q := \{(0, 0), \dots, (q-1, 0)\} \subset \mathbb{R}^2.$$

Hence, every point in the crystal can be uniquely represented as

$$\tilde{\eta} + \underline{x}, \quad \tilde{\eta} \in \Gamma_q, \underline{x} \in \mathcal{Y}_q,$$

where

$$\tilde{\eta} = (q\eta_1, \eta_2), \quad \eta_1, \eta_2 \in \mathbb{Z}, \quad \underline{x} = \underline{y} + \underline{z}, \quad \underline{z} \in \mathcal{B}_q, \underline{y} \in \mathcal{Y}.$$

In the following, we will often naturally identify $\tilde{\eta} = (q\eta_1, \eta_2) \in \Gamma_q$ with $\eta = (\eta_1, \eta_2) \in \mathbb{Z}^2$, and correspondingly identify e.g. the magnetic phases $e^{i\phi(\tilde{\eta}, \tilde{\eta}')} = e^{iq\phi(\eta, \eta')}$ or, with a little abuse of notation, the matrix elements $\mathcal{T}((q\eta_1, \eta_2); \underline{x}) = \mathcal{T}(\tilde{\eta} + \underline{z}; \underline{y})$.

With this notation, we then have following result:

Proposition 5.2.1. *Assume that $b_0 q \in 2\pi\mathbb{Z}$ as above. Set $Q = Q(q) := qN$. Then, for every $\epsilon \geq 0$, there exists a family of $Q \times Q$ self-adjoint matrices $h_{\mathbf{k}, b_0 + \epsilon}$ which is real-analytic and \mathbb{Z}^2 -periodic as a function of \mathbf{k} , real-analytic as a function of ϵ , and*

such that $H_{b_0+\epsilon}$ is unitarily equivalent via a unitary operator $U_{b_0+\epsilon}$ to an operator in $\ell^2(\mathbb{Z}^2) \otimes \mathbb{C}^Q$ given by the matrix elements

$$\begin{aligned} \tilde{\mathcal{H}}_\epsilon(\gamma, \underline{x}; \gamma', \underline{x}') &:= e^{i\epsilon q \phi(\gamma, \gamma')} \mathcal{T}_\epsilon(\gamma - \gamma'; \underline{x}, \underline{x}'), \\ \text{where } \mathcal{T}_\epsilon(\gamma; \underline{x}, \underline{x}') &:= \int_{\Omega} d\mathbf{k} e^{i2\pi \mathbf{k} \cdot \gamma} h_{\mathbf{k}, b_0+\epsilon}(\underline{x}, \underline{x}'), \end{aligned} \quad (5.2.3)$$

with $\gamma, \gamma' \in \mathbb{Z}^2$ and $\underline{x}, \underline{x}' \in \{1, \dots, Q\}$.

Proof. Write $b_0 = 2\pi p/q$ with $p, q \in \mathbb{Z}$ coprime, and let $b = b_0 + \epsilon$, where $\epsilon > 0$. Define the unitary operator from $\ell^2(\mathbb{Z}^2) \otimes \ell^2(\mathcal{Y})$ to $\ell^2(\Gamma_q) \otimes \ell^2(\mathcal{Y}_q)$ acting on $f \in \ell^2(\mathbb{Z}^2) \otimes \ell^2(\mathcal{Y})$ by

$$\begin{aligned} [U_b f](\tilde{\eta}, \underline{x}) &:= e^{ib_0 \tilde{\eta}_1 \tilde{\eta}_2 / 2} e^{ib\phi(\tilde{\eta}, \underline{x})} f(\tilde{\eta} + \underline{z}, \underline{y}) \\ &= e^{i\pi p \eta_1 \eta_2} e^{ib\phi(\tilde{\eta}, \underline{x})} f(\tilde{\eta} + \underline{z}, \underline{y}) \quad \tilde{\eta} \in \Gamma_q, \underline{x} \in \mathcal{Y}_q, \end{aligned} \quad (5.2.4)$$

where we have used the unique decomposition $\mathcal{Y}_q \ni \underline{x} = \underline{y} + \underline{z}$, $\underline{z} \in \mathcal{B}_q$, $\underline{y} \in \mathcal{Y}$. We note the identity

$$\phi(\tilde{\eta} + \underline{x}, \tilde{\eta}' + \underline{x}') = \phi(\tilde{\eta}, \tilde{\eta}') + \phi(\tilde{\eta} - \tilde{\eta}', \underline{x} + \underline{x}') + \phi(\underline{x}, \underline{x}') + \phi(\underline{x}, \tilde{\eta}) - \phi(\underline{x}', \tilde{\eta}').$$

By rotating H_b with U_b we have

$$\begin{aligned} [U_b H_b U_b^*](\tilde{\eta}, \underline{x}; \tilde{\eta}', \underline{x}') &= e^{i\epsilon \phi(\tilde{\eta}, \tilde{\eta}')} e^{ib_0 \tilde{\eta}'_1 (\tilde{\eta}_2 - \tilde{\eta}'_2)} e^{ib_0 (\tilde{\eta}_1 - \tilde{\eta}'_1) (\tilde{\eta}_2 - \tilde{\eta}'_2) / 2} \\ &\quad \cdot e^{ib\phi(\tilde{\eta} - \tilde{\eta}', \underline{x} + \underline{x}')} e^{ib\phi(\underline{x}, \underline{x}')} \mathcal{T}(\tilde{\eta} - \tilde{\eta}'; \underline{x}, \underline{x}'). \end{aligned}$$

We observe that $b_0 \tilde{\eta}'_1 (\tilde{\eta}_2 - \tilde{\eta}'_2) = 2\pi p \eta'_1 (\eta_2 - \eta'_2) \in 2\pi \mathbb{Z}$, thus $e^{ib_0 \tilde{\eta}'_1 (\tilde{\eta}_2 - \tilde{\eta}'_2)} = 1$ and

$$\begin{aligned} (\tilde{\eta}, \underline{x}; \tilde{\eta}', \underline{x}') &= e^{i\epsilon \phi(\tilde{\eta}, \tilde{\eta}')} (-1)^{p(\eta_1 - \eta'_1)(\eta_2 - \eta'_2)} \\ &\quad \cdot e^{ib\phi(\tilde{\eta} - \tilde{\eta}', \underline{x} + \underline{x}')} e^{ib\phi(\underline{x}, \underline{x}')} \mathcal{T}(\tilde{\eta} - \tilde{\eta}'; \underline{x}, \underline{x}'). \end{aligned}$$

Upon the identification of $\tilde{\gamma} = (q\gamma_1, \gamma_2) \in \Gamma_q$ with $\gamma = (\gamma_1, \gamma_2) \in \mathbb{Z}^2$ as in the comments before the statement, every operator on $\ell^2(\Gamma_q) \otimes \ell^2(\mathcal{Y}_q)$ is identified with an operator on $\ell^2(\mathbb{Z}^2) \otimes \ell^2(\mathcal{Y}_q)$. In particular, the above unitary conjugation of the Hofstadter-like Hamiltonian can be seen as acting in $\ell^2(\mathbb{Z}^2) \otimes \ell^2(\mathcal{Y}_q)$ with matrix elements

$$\begin{aligned} \tilde{\mathcal{H}}_\epsilon(\gamma, \underline{x}; \gamma', \underline{x}') &:= e^{i\epsilon q \phi(\gamma, \gamma')} (-1)^{p(\gamma_1 - \gamma'_1)(\gamma_2 - \gamma'_2)} e^{i(b_0 + \epsilon)(\gamma_2 - \gamma'_2)(\underline{x}_1 + \underline{x}'_1) / 2} \\ &\quad \cdot e^{-iq(b_0 + \epsilon)(\gamma_1 - \gamma'_1)(\underline{x}_2 + \underline{x}'_2) / 2} e^{i(b_0 + \epsilon)\phi(\underline{x}, \underline{x}')} \\ &\quad \cdot \mathcal{T}((q(\gamma_1 - \gamma'_1), \gamma_2 - \gamma'_2); \underline{x}, \underline{x}'). \end{aligned} \quad (5.2.5)$$

Notice that the whole expression on the right-hand side of the above, with the exception of the phase $e^{i\epsilon q \phi(\gamma, \gamma')}$, depends only on the difference $\gamma - \gamma'$. Identifying $\ell^2(\mathcal{Y}_q) \simeq \ell^2(\mathcal{B}_q) \otimes \ell^2(\mathcal{Y}) \simeq \mathbb{C}^q \otimes \mathbb{C}^N \simeq \mathbb{C}^{qN}$, we can thus determine a new Bloch fiber for $\tilde{\mathcal{H}}_\epsilon$, which will be a matrix of size $qN \times qN$ equal to

$$\begin{aligned} h_{\mathbf{k}, b_0+\epsilon}(\underline{x}; \underline{x}') &:= \sum_{\gamma \in \mathbb{Z}^2} e^{-i2\pi \mathbf{k} \cdot \gamma} (-1)^{p\gamma_1 \gamma_2} e^{i(\pi p/q + \epsilon/2)\gamma_2(\underline{x}_1 + \underline{x}'_1)} \\ &\quad \cdot e^{-i(\pi p + q\epsilon/2)\gamma_1(\underline{x}_2 + \underline{x}'_2)} e^{i(b_0 + \epsilon)\phi(\underline{x}, \underline{x}')} \mathcal{T}((q\gamma_1, \gamma_2); \underline{x}, \underline{x}'). \end{aligned}$$

Moreover, the family of matrices $h_{\mathbf{k}, b_0+\epsilon}$ is real-analytic in both \mathbf{k} and ϵ . This is a simple direct consequence of the exponential decay of $\mathcal{T}(\gamma)$ as a function of γ , which in turn is a consequence of the real-analyticity in \mathbf{k} of the original $h_{\mathbf{k}}$. \square

Let us now use the above result to show how the original rational flux Hamiltonian H_{b_0} is unitarily equivalent to a fibered operator. Indeed, if $\epsilon = 0$, the Hamiltonian $\tilde{\mathcal{H}}_0$ is periodic, that is, it commutes with the usual translation operators by shifts in \mathbb{Z}^2 . Therefore, it is possible to diagonalize it by using the usual Bloch–Floquet theory [98, 69, 49, 71]. Consider the Bloch–Floquet transform \mathcal{U}_{BF} defined, for every $f \in C_0^\infty(\mathbb{Z}^2) \otimes \ell^2(\mathcal{Y}_q)$, as

$$(\mathcal{U}_{\text{BF}}f)_{\mathbf{k}}(\underline{x}) := \sum_{\eta \in \mathbb{Z}^2} e^{-i2\pi\mathbf{k}\cdot\eta} f(\eta, \underline{x}), \quad \mathbf{k} \in \Omega, \underline{x} \in \mathcal{Y}_q,$$

and then extended by continuity to a unitary operator $\mathcal{U}_{\text{BF}}: \ell^2(\mathbb{Z}^2) \otimes \ell^2(\mathcal{Y}_q) \rightarrow L^2(\Omega) \otimes \ell^2(\mathcal{Y}_q)$.

Let us introduce the group of (*modified*) *magnetic translations* $\hat{\tau}_{b_0, \tilde{\eta}}$ defined for every $\tilde{\eta} \in \Gamma_q$ by

$$[\hat{\tau}_{b_0, \tilde{\eta}}f](\tilde{\gamma}, \underline{x}) := e^{ib_0\tilde{\eta}_1\tilde{\eta}_2/2} e^{ib_0\phi(\tilde{\gamma}+\underline{x}, \tilde{\eta})} f(\tilde{\gamma} - \tilde{\eta}, \underline{x}), \quad f \in \ell^2(\Gamma_q) \otimes \ell^2(\mathcal{Y}_q). \quad (5.2.6)$$

We stress that the phase factor $e^{ib_0\tilde{\eta}_1\tilde{\eta}_2/2}$ is crucial in order to have a *unitary representation* of the group \mathbb{Z}^2 (that is, $\hat{\tau}_{b_0, \tilde{\eta}}\hat{\tau}_{b_0, \tilde{\gamma}} = \hat{\tau}_{b_0, \tilde{\eta}+\tilde{\gamma}}$ for $\tilde{\gamma}, \tilde{\eta} \in \Gamma_q$), instead of just a projective one (compare Remark 5.2.2 below), when $b_0 \in 2\pi\mathbb{Q}$.

Define the following operator:

$$\begin{aligned} (\mathcal{U}_{\text{mBF}}g)_{\mathbf{k}}(\underline{x}) &:= (\mathcal{U}_{\text{BF}}U_{b_0}g)_{\mathbf{k}}(\underline{x}) \\ &= \sum_{\eta \in \mathbb{Z}^2} e^{-i2\pi\mathbf{k}\cdot\eta} (\hat{\tau}_{b_0, -(q\eta_1, \eta_2)}g)(0, \underline{x}), \quad g \in C_0^\infty(\mathbb{Z}^2) \otimes \ell^2(\mathcal{Y}). \end{aligned} \quad (5.2.7)$$

The unitary operator \mathcal{U}_{mBF} is a modified Bloch–Floquet transform. Then we have the identity

$$\mathcal{U}_{\text{BF}}\tilde{\mathcal{H}}_0\mathcal{U}_{\text{BF}}^* = \mathcal{U}_{\text{mBF}}H_{b_0}\mathcal{U}_{\text{mBF}}^* = \int_{\Omega}^{\oplus} d\mathbf{k} h(\mathbf{k}), \quad (5.2.8)$$

where the fiber Hamiltonian $h(\mathbf{k}) \equiv h_{\mathbf{k}, b_0}$ is periodic in \mathbf{k} with respect to shifts in the dual lattice $\{\mathbf{k} \in \mathbb{R}^2 : \mathbf{k} \cdot \eta \in 2\pi\mathbb{Z} \forall \eta \in \mathbb{Z}^2\} \simeq \mathbb{Z}^2$ and acts on functions with fixed crystal momentum \mathbf{k} , so only on the degrees of freedom in the supercell \mathcal{Y}_q .

If the Hamiltonian H_{b_0} is gapped, then its Fermi projection Π_{b_0} onto the (finite) gapped spectral island is also unitarily equivalent to a direct integral $\int_{\mathbb{T}^2}^{\oplus} d\mathbf{k} P(\mathbf{k})$ of (finite-rank) projections, and the same properties of regularity and periodicity in \mathbf{k} claimed in Proposition 5.2.1 for the fibers $h(\mathbf{k})$ hold for $P(\mathbf{k})$ as well.

While the original Hamiltonian H_{b_0} commutes with the modified magnetic translations defined in (5.2.6), we stress, once again, that the Hamiltonian $\tilde{\mathcal{H}}_0$ is truly a periodic operator. Indeed, $\tilde{\mathcal{H}}_0$ commutes with the usual translations defined, for every $f \in \ell(\mathbb{Z}^2) \otimes \mathbb{C}^Q$, by

$$[\tau_{0, \eta}f](\gamma, \underline{x}) := f(\gamma - \eta, \underline{x}), \quad \eta \in \mathbb{Z}^2.$$

This is reflected by (5.2.8), where $\tilde{\mathcal{H}}_0$ is fibered by the Bloch–Floquet transform \mathcal{U}_{BF} . The situation is different when we consider an irrational magnetic flux. Indeed, the original perturbed Hamiltonian $H_{b_0+\epsilon}$ commutes with the magnetic translations

associated to $b_0 + \epsilon$, that is the unitary operator defined, for every $f \in \ell(\mathbb{Z}^2) \otimes \ell(\mathcal{Y})$, by

$$[\tau_\eta^{(b_0+\epsilon)} f](\gamma, \underline{x}) := e^{i(b_0+\epsilon)\phi(\gamma+\underline{x}, \eta)} f(\gamma - \eta, \underline{x}), \quad \eta \in \mathbb{Z}^2. \quad (5.2.9)$$

Instead, because of the action of the unitary operator $U_{b_0+\epsilon}$, the Hamiltonian $\tilde{\mathcal{H}}_\epsilon$ commutes with the unitary operator defined, for every $f \in \ell(\mathbb{Z}^2) \otimes \mathbb{C}^Q$, by

$$[\tau_{\epsilon, \eta} f](\gamma, \underline{x}) := e^{i\epsilon q \phi(\gamma, \eta)} f(\gamma - \eta, \underline{x}), \quad \eta \in \mathbb{Z}^2. \quad (5.2.10)$$

Remark 5.2.2. More generally, notice that any operator A on $\ell^2(\mathbb{Z}^2) \otimes \mathbb{C}^Q$ whose matrix elements are of the form

$$A(\gamma, \underline{x}; \gamma', \underline{x}') := e^{i\epsilon q \phi(\gamma, \gamma')} a_\epsilon(\gamma - \gamma'; \underline{x}, \underline{x}'), \quad \gamma, \gamma' \in \mathbb{Z}^2, \underline{x}, \underline{x}' \in \{1, \dots, Q\},$$

commutes with the magnetic translations $\tau_{\epsilon, \eta}$, $\eta \in \mathbb{Z}^2$, defined in (5.2.10). Indeed for $f \in \ell^2(\mathbb{Z}^2) \otimes \mathbb{C}^Q$

$$\begin{aligned} [A\tau_{\epsilon, \eta} f](\gamma, \underline{x}) &= \sum_{\gamma' \in \mathbb{Z}^2} \sum_{\underline{x}'=1}^Q e^{i\epsilon q \phi(\gamma, \gamma')} a_\epsilon(\gamma - \gamma'; \underline{x}, \underline{x}') e^{i\epsilon q \phi(\gamma', \eta)} f(\gamma' - \eta, \underline{x}') \\ &= \sum_{\gamma'' = \gamma' - \eta \in \mathbb{Z}^2} \sum_{\underline{x}'=1}^Q e^{i\epsilon q \phi(\gamma, \gamma'' + \eta)} a_\epsilon(\gamma - \gamma'' + \eta; \underline{x}, \underline{x}') e^{i\epsilon q \phi(\gamma'' + \eta, \eta)} f(\gamma'', \underline{x}') \\ &= e^{i\epsilon q \phi(\gamma, \eta)} \sum_{\gamma'' \in \mathbb{Z}^2} \sum_{\underline{x}'=1}^Q e^{i\epsilon q \phi(\gamma - \eta, \gamma'')} a_\epsilon(\gamma - \eta - \gamma''; \underline{x}, \underline{x}') f(\gamma'', \underline{x}') \\ &= [\tau_{\epsilon, \eta} A f](\gamma, \underline{x}), \end{aligned} \quad (5.2.11)$$

where we repeatedly used the skew-symmetry of the Peierls magnetic phase $\phi(\cdot, \cdot)$.

Contrary to the modified magnetic translations $\hat{\tau}_{b_0, \eta}$ defined in (5.2.6), the translation operators $\tau_{\epsilon, \eta}$ do not form a unitary representation of the group \mathbb{Z}^2 , but rather a projective one. Indeed

$$\tau_{\epsilon, \eta}^* = \tau_{\epsilon, -\eta} \quad \text{and} \quad \tau_{\epsilon, \eta} \tau_{\epsilon, \eta'} = e^{i\epsilon q \phi(\eta', \eta)} \tau_{\epsilon, \eta + \eta'}, \quad \eta, \eta' \in \mathbb{Z}^2. \quad (5.2.12)$$

The main achievement of Proposition 5.2.1 is to reduce the original Hamiltonian $H_{b_0+\epsilon}$ to the product of a phase factor times a fibered operator, that is \mathcal{T}_ϵ , whose fiber $h_{\mathbf{k}, b_0+\epsilon}$ acts in a fiber space whose dimension Q is independent of ϵ and which only depends on b_0 via q . This is crucial in order to control the perturbation induced by ϵ , because the ϵ -dependent fiber operators act in the *same* space even as ϵ is varying. Even though the representation in Proposition 5.2.1 is valid for all values of ϵ , it will be used for ϵ sufficiently small, for which the spectral properties of H_{b_0} and $H_{b_0+\epsilon}$ are “comparable” (i.e., for which the spectral gap of the rational-flux Hamiltonian persists also at $\epsilon \neq 0$).

5.3 Periodic setting: results for rational flux Hamiltonians

Having established a clear reference model, we now abstract from the periodic setting of Hofstadter-like Hamiltonians satisfying a rational flux condition, and consider

families of rank- m orthogonal projections $\{P(\mathbf{k})\}_{\mathbf{k} \in \mathbb{R}^d}$, $P(\mathbf{k}) = P(\mathbf{k})^2 = P(\mathbf{k})^*$, acting on some Hilbert space \mathcal{H} , which are subject to the following conditions:

- (i) the map $P: \mathbb{R}^d \rightarrow \mathcal{B}(\mathcal{H})$, $\mathbf{k} \mapsto P(\mathbf{k})$, is smooth (at least of class C^1);
- (ii) the map $P: \mathbb{R}^d \rightarrow \mathcal{B}(\mathcal{H})$, $\mathbf{k} \mapsto P(\mathbf{k})$, is \mathbb{Z}^d -periodic, that is, $P(\mathbf{k}) = P(\mathbf{k} + \mathbf{n})$ for all $\mathbf{n} \in \mathbb{Z}^d$.

The rank m corresponds to the number of occupied energy bands in physical applications. As discussed e.g. in [30, 79], the same setting arises also from continuous models (described by a magnetic Schrödinger operator as the Hamiltonian) of gapped periodic quantum systems subject to a magnetic field satisfying the rational flux property: we note that, in this case, some technical modifications are required to define the Bloch–Floquet representation, and one is led to use in this case the so-called (*magnetic*) *Bloch–Floquet–Zak transform* (see also [49]).

Definition 5.3.1. A *Bloch vector* for the family of projections $\{P(\mathbf{k})\}_{\mathbf{k} \in \mathbb{R}^d}$ is a map $\xi: \mathbb{R}^d \rightarrow \mathcal{H}$ such that

$$P(\mathbf{k})\xi(\mathbf{k}) = \xi(\mathbf{k}) \quad \text{for all } \mathbf{k} \in \mathbb{R}^d.$$

A Bloch vector ξ is called

- (i) *continuous* if the map $\xi: \mathbb{R}^d \rightarrow \mathcal{H}$ is continuous;
- (ii) *periodic* if the map $\xi: \mathbb{R}^d \rightarrow \mathcal{H}$ is \mathbb{Z}^d -periodic, that is, $\xi(\mathbf{k}) = \xi(\mathbf{k} + \mathbf{n})$ for all $\mathbf{n} \in \mathbb{Z}^d$;
- (iii) *normalized* if $\|\xi(\mathbf{k})\| = 1$ for all $\mathbf{k} \in \mathbb{R}^d$.

A collection of M Bloch vectors $\{\xi_a\}_{a=1}^M$ is said to be

- (i) *independent* (respectively *orthonormal*) if the vectors $\{\xi_a(\mathbf{k})\}_{a=1}^M \subset \mathcal{H}$ are linearly independent (respectively orthonormal) for all $\mathbf{k} \in \mathbb{R}^d$;
- (ii) a *moving Parseval M -frame* (or *M -frame* in short) if $M \geq m$ and for every $\psi \in \text{Ran } P(\mathbf{k})$ we have

$$\psi = \sum_{a=1}^M \langle \xi_a(\mathbf{k}), \psi \rangle \xi_a(\mathbf{k}) \quad \text{or equivalently} \quad \|\psi\|^2 = \sum_{a=1}^M |\langle \xi_a(\mathbf{k}), \psi \rangle|^2. \quad (5.3.1)$$

If $M = m$, we call $\{\xi_a\}_{a=1}^m$ a *Bloch basis*.

In general, all the above conditions on a collection of Bloch vectors compete against each other, and one has to give up some of them in order to enforce the others. As was recalled in the Introduction, this is well-known in differential geometry. Indeed, given a smooth, periodic family of projections, one can construct the associated *Bloch bundle* $\mathcal{E} \rightarrow \mathbb{T}^d$ [89], which is an Hermitian vector bundle over the (Brillouin) d -torus $\mathbb{T}^d = \mathbb{R}^d / \mathbb{Z}^d$, and Bloch vectors are nothing but *sections* for this vector bundle. The *topological obstruction* to construct sections of a vector bundle reflects in the impossibility to construct collections of Bloch vectors with the required properties. For example:

- in general, a Bloch vector can be continuous but *not* periodic, or viceversa periodic but *not* continuous: in the latter case, one then speaks of *local sections* of the associated Bloch bundle, defined in the patches where they are continuous;
- global (continuous and periodic) sections may exist, but they may *vanish* in \mathbb{T}^d , thus violating the normalization condition for a Bloch vector;
- when $d \leq 3$, the topological obstruction to construct a (possibly orthonormal) Bloch basis consisting of continuous, periodic Bloch vectors is encoded in the *Chern numbers* [4, 89, 76]

$$c_1(P)_{ij} = \frac{1}{2\pi i} \int_{\mathbb{T}_{ij}^2} dk_i dk_j \operatorname{Tr}_{\mathcal{H}} (P(\mathbf{k}) [\partial_i P(\mathbf{k}), \partial_j P(\mathbf{k})]) \in \mathbb{Z}, \quad 1 \leq i < j \leq d, \quad (5.3.2)$$

where $\mathbb{T}_{ij}^2 \subset \mathbb{T}^d$ is the 2-torus where the coordinates different from k_i and k_j are set equal to zero. Only when the Chern numbers vanish does a Bloch basis exist, in which case the Bloch bundle is *trivial*, i.e. isomorphic to $\mathbb{T}^d \times \mathbb{C}^m$.

In the first part of this chapter, we discuss the possibility of relaxing the condition to be a continuous, periodic, and orthonormal Bloch basis in two possible ways, by considering instead collections of M Bloch vectors such that

- (i) $M < m$, and the continuous, periodic Bloch vectors are still *orthonormal*;
- (ii) $M > m$, and the continuous, periodic Bloch vectors are still *generating* (hence constitute an M -frame).

In the present context of families of projections arising from gapped crystalline Hamiltonians, optimal *existence* results on orthonormal sets and Parseval frames of Bloch vectors were first proved in [70, 3] via general bundle-theoretic argument, as already mentioned in Section 5.1.1. Here “optimal” refers to finding the optimal value M in each of the two situations (the maximal M in the first, and the minimal M in the second). The results are summarized in the following

Theorem 5.3.2 ([3, 70]). *Let $d \leq 3$, and let $\{P(\mathbf{k})\}_{\mathbf{k} \in \mathbb{R}^d}$ be a smooth, \mathbb{Z}^d -periodic family of orthogonal projections of rank m .*

- (i) *There exist at least $m - 1$ independent Bloch vectors which are continuous and \mathbb{Z}^d -periodic.*
- (ii) *There exists a Parseval $(m + 1)$ -frame of continuous and \mathbb{Z}^d -periodic Bloch vectors (see (5.3.1)).*
- (iii) *Assume furthermore that $c_1(P)_{ij} = 0 \in \mathbb{Z}$ for all $1 \leq i < j \leq d$, where $c_1(P)_{ij}$ is defined in (5.3.2). Then, there exists an orthonormal Bloch basis of continuous and \mathbb{Z}^d -periodic Bloch vectors.*

Remark 5.3.3. By standard arguments, which we reproduce in Appendix A.2.1 for the reader’s convenience, it is possible to improve the regularity of Bloch vectors if the family of projections is more regular: the only obstruction is to continuity. In other

words, if for example the map $\mathbf{k} \mapsto P(\mathbf{k})$ is smooth or analytic, then a continuous Bloch vector yields a smooth or real-analytic one by convolution with a sufficiently regular kernel. Moreover, one can always make sure that all the other properties (periodicity, orthogonality, ...) are preserved by this smoothing procedure.

As was already remarked in Section 5.1.1, in the case of an analytic family of projections the techniques of [3, 70] allow to show the existence of Bloch vectors which are analytic in the same analyticity strip. The explicit smoothing procedure mentioned above, instead, only gives a weaker real analyticity (i.e. analyticity of the Bloch vectors in a complex strip around the real \mathbf{k} 's of *a priori* smaller width than the one of the analyticity domain of the projections).

Abstract results concerning the existence of such collections of Bloch vectors can be also found in the literature on vector bundles. For example:

- (i) by [63, Chap. 9, Thm. 1.2], there exist $m - \ell_d$ continuous and periodic *independent* sections of the Bloch bundle, where ² $\ell_d = \lceil (d-1)/2 \rceil$;
- (ii) by [63, Chap. 8, Thm. 7.2], there exists an $(m+r_d)$ -*frame* for the Bloch bundle, where $r_d = \lceil d/2 \rceil$.

The second of the above statements can be rephrased by saying that there exists a *trivial* vector bundle \mathcal{F} of rank $m+r_d$ that contains \mathcal{E} as a subbundle. Indeed, if $\{\psi_a\}_{a=1}^{m+r_d}$ is a moving basis for \mathcal{F} , then setting $\xi_a(\mathbf{k}) := P(\mathbf{k})\psi_a(\mathbf{k})$, $a \in \{1, \dots, m+r_d\}$, defines an $(m+r_d)$ -*frame* for \mathcal{E} (see also [48]). Notice that the above Theorem 5.3.2 for $d=3$ yields an optimal number ($M = m+1$) of vectors in a Parseval frame, which is actually smaller than the number $M = m+r_{d=3} = m+2$ predicted by the general, bundle-theoretic result quoted above [63, Chap. 8, Thm. 7.2].

This kind of results have a much broader range of applicability and hold for a large class of base manifolds (of which the base space of the Bloch bundle, namely the d -torus for $d \leq 3$, is only a very specific case). However, their proofs rely on techniques from algebraic topology, specifically on homotopy and obstruction theory, which may not be particularly suited to numerical implementations, because for example they allow to construct the required objects only up to homotopies which are often difficult to describe analytically.

Aiming at this type of applications in computational condensed matter physics, as already mentioned in the Introduction (see also Section 5.3.2 below), our first contribution in this direction is to provide an *alternative, algorithmic proof* of Theorem 5.3.2, which explicitly exhibits the optimal number of orthonormal (respectively generating) Bloch vectors via an algorithm, in a finite number of steps and working out all analytical details (mostly in the Appendices and in references therein). The algorithm we propose is sketched at the end of the next section, and the details of our proof of Theorem 5.3.2 are presented in Sections 5.5 to 5.7.

5.3.1 Applications to Wannier functions

Concerning the specific case of Bloch bundles arising from condensed matter systems, the construction of (real-analytic) Bloch vectors translates to the construction of

²We denote by $\lceil x \rceil$ the smallest integer n such that $x \leq n$.

localized (composite) Wannier functions for the occupied states of the magnetic Hamiltonian describing the crystal, by transforming the Bloch vectors back from the \mathbf{k} -space representation to the position representation via the Bloch–Floquet transform (5.1.1) [71]. Our proof of the second part of Theorem 5.3.2 can then be rephrased as the possibility to *algorithmically construct* Parseval frames for the spectral island onto m gapped energy bands consisting of $m + 1$ exponentially localized Wannier functions, together with their (magnetic) translates. Although, as mentioned above, the range of applicability of Theorem 5.3.2 on Bloch vectors includes also spectral projections of certain magnetic Schrödinger operators, for simplicity, and in order to avoid too many technical conditions, we only formulate the result for Hofstadter-like Hamiltonians:

Theorem 5.3.4. *Let H_{b_0} be an Hofstadter-like Hamiltonian on $\ell^2(\mathbb{Z}^2) \otimes \ell^2(\mathcal{Y})$ corresponding to a magnetic field $b_0 \in 2\pi\mathbb{Q}$. Let $\Pi = \Pi_{b_0}$ be the spectral projection onto an isolated spectral island of H_{b_0} consisting of m energy bands, and let $\mathcal{U}_{mBF} \Pi \mathcal{U}_{mBF}^* = \int_{\mathbb{T}^2}^{\oplus} d\mathbf{k} P(\mathbf{k})$. Then:*

- (i) *there exists an exponentially localized Wannier Parseval frame for the subspace $\text{Ran } \Pi \subset \ell^2(\mathbb{Z}^2) \otimes \ell^2(\mathcal{Y})$, i.e. there exist $m + 1$ exponentially localized vectors w_a , $a \in \{1, \dots, m + 1\}$, such that*

$$w = \sum_{\gamma \in \mathbb{Z}^2} \sum_{a=1}^{m+1} \langle \hat{\tau}_{b_0, \gamma} w_a, w \rangle (\hat{\tau}_{b_0, \gamma} w_a) \quad \text{for all } w \in \text{Ran } \Pi;$$

- (ii) *if moreover $c_1(P) = 0 \in \mathbb{Z}$, where $c_1(P) \equiv c_1(P)_{12}$ is defined in (5.3.2), then there exist m exponentially localized vectors w_a , $a \in \{1, \dots, m\}$, such that $\{\hat{\tau}_{b_0, \gamma} w_a\}_{a \in \{1, \dots, m\}, \gamma \in \mathbb{Z}^2}$ is an orthonormal basis of $\text{Ran } \Pi \subset \ell^2(\mathbb{Z}^2) \otimes \ell^2(\mathcal{Y})$.*

We stress again that, using our proof of Theorem 5.3.2, the objects whose existence is claimed in Theorem 5.3.4 can be constructed with a finite-step algorithm that in principle can be numerically implemented.

5.3.2 Why are Parseval frames useful in solid state physics?

Inspired by [70], we advocate the use of Parseval frames of localized Wannier functions as an efficient tool to derive tight-binding models for magnetic Hamiltonians, much in the same way as orthonormal bases are used in topologically unobstructed cases, e.g. under a time-reversal symmetry assumption [89, 77].

To substantiate this claim let us start by some general considerations, and recall the definition of a classical Parseval Gabor frame [59, 107]. For every pair $(\lambda, \gamma) \in \mathbb{Z}^d \times \mathbb{Z}^d = \mathbb{Z}^{2d}$ we consider the functions $\psi_{\lambda\gamma}(\mathbf{x}) := e^{2\pi i \lambda \cdot \mathbf{x}} g(\mathbf{x} - \gamma)$ where g is a smooth function, compactly supported in $[-1, 1]^d$ and such that $\sum_{\gamma \in \mathbb{Z}^d} |g(\mathbf{x} - \gamma)|^2 = 1$ for all $\mathbf{x} \in \mathbb{R}^d$. It is well-known that the set $\{\psi_{\lambda\gamma}\}_{\lambda, \gamma \in \mathbb{Z}^d}$ forms an overcomplete Parseval frame in $L^2(\mathbb{R}^d)$, in the sense that any $f \in L^2(\mathbb{R}^d)$ can be written as

$$f = \sum_{\lambda, \gamma \in \mathbb{Z}^d} \langle \psi_{\lambda\gamma}, f \rangle \psi_{\lambda\gamma}, \quad \text{with} \quad \|f\|^2 = \sum_{\lambda, \gamma \in \mathbb{Z}^d} |\langle \psi_{\lambda\gamma}, f \rangle|^2.$$

Although a Parseval frame is not an orthonormal basis, one can represent any reasonable linear (pseudo-differential) operator A on $L^2(\mathbb{R}^d)$ as an “infinite double

matrix" acting in $\ell^2(\mathbb{Z}^{2d})$, where the matrix elements are given by $A(\lambda, \gamma; \lambda', \gamma') := \langle \psi_{\lambda\gamma}, A\psi_{\lambda'\gamma'} \rangle$ [57, 45].

In applications one is typically interested in finding a generating set of vectors for the subspace which is the range of an orthogonal Fermi projection Π onto an isolated group of m bands of an Hamiltonian H unitarily conjugated to a fibered operator $\int_{\mathbb{T}^d}^{\oplus} d\mathbf{k} h(\mathbf{k})$. Our proof of Theorem 5.3.4 provides a way to construct the *smallest* finite set of *exponentially* localized functions $\{w_a\}_{1 \leq a \leq M}$ with $m \leq M$ such that

$$\Pi = \sum_{\gamma \in \mathbb{Z}^d} \sum_{a=1}^M |T_\gamma w_a\rangle \langle T_\gamma w_a|$$

where $\gamma \mapsto T_\gamma$ is a suitable representation of the translation group \mathbb{Z}^d (e.g. $T_\gamma = \hat{\tau}_{b_0, \gamma}$ for rational-flux Hofstadter-like Hamiltonians in $d = 2$). In particular, the existence of a Parseval frame allows to isometrically identify $\text{Ran } \Pi$ with the space $\ell^2(\mathbb{Z}^d) \otimes \mathbb{C}^M$. The number M is either m or $m + 1$, depending on the vanishing or not of the Chern numbers of the Bloch bundle associated to the fibers $\{P(\mathbf{k})\}_{\mathbf{k} \in \mathbb{T}^d}$ of Π .

The analytic and periodic Bloch frame corresponding to the Parseval frame $\{T_\gamma w_a\}_{1 \leq a \leq M, \gamma \in \mathbb{Z}^d}$, see Theorem 5.3.2, can be also used to construct an effective model to study, for example, the band structure of the fiber Bloch Hamiltonian $h(\mathbf{k})$ numerically through Fourier interpolation [116, 74]. By the gap condition and a shift of the (Fermi) energy, we can assume that $h(\mathbf{k})$ has a gap at zero energy and hence has non-zero eigenvalues. Denote by $E_j(\mathbf{k}) \neq 0$ the Bloch energy bands, labelled in increasing order, and by $\psi_j(\mathbf{k})$ the corresponding (normalized) Bloch eigenfunctions, $h(\mathbf{k})\psi_j(\mathbf{k}) = E_j(\mathbf{k})\psi_j(\mathbf{k})$. Assume that the negative eigenvalues (below the spectral gap and the Fermi energy) are labelled by $j \in \{1, \dots, m\}$. We have

$$P(\mathbf{k}) = \sum_{j=1}^m |\psi_j(\mathbf{k})\rangle \langle \psi_j(\mathbf{k})|, \quad h(\mathbf{k})P(\mathbf{k}) = \sum_{j=1}^m E_j(\mathbf{k}) |\psi_j(\mathbf{k})\rangle \langle \psi_j(\mathbf{k})|.$$

The eigenvectors $\psi_j(\mathbf{k})$ are not necessarily smooth in \mathbf{k} even though $h(\mathbf{k})P(\mathbf{k})$ is smooth and periodic. Using our Parseval frame $\{\xi_a(\mathbf{k})\}_{1 \leq a \leq M}$ as in (5.3.1), we can introduce an $M \times M$ matrix $h_{\text{eff}}(\mathbf{k})$ acting on \mathbb{C}^M and given by

$$h_{\text{eff}}(\mathbf{k})_{aa'} := \langle \xi_a(\mathbf{k}), h(\mathbf{k})\xi_{a'}(\mathbf{k}) \rangle_{\mathcal{H}}, \quad 1 \leq a, a' \leq M.$$

This matrix is both smooth and periodic; we show further that its non-zero spectrum coincides with the relevant Bloch eigenvalues $E_j(\mathbf{k})$. Define the vectors $\Psi_j(\mathbf{k}) \in \mathbb{C}^M$, $j \in \{1, \dots, m\}$, with components given by $(\Psi_j(\mathbf{k}))_a = \langle \xi_a(\mathbf{k}), \psi_j(\mathbf{k}) \rangle_{\mathcal{H}}$, $a \in \{1, \dots, M\}$. Then, by the Parseval property (5.3.1),

$$\langle \Psi_j(\mathbf{k}), \Psi_{j'}(\mathbf{k}) \rangle_{\mathbb{C}^M} = \sum_{a=1}^M \langle \psi_j(\mathbf{k}), \xi_a(\mathbf{k}) \rangle_{\mathcal{H}} \langle \xi_a(\mathbf{k}), \psi_{j'}(\mathbf{k}) \rangle_{\mathcal{H}} = \langle \psi_j(\mathbf{k}), \psi_{j'}(\mathbf{k}) \rangle_{\mathcal{H}} = \delta_{jj'}$$

and furthermore, by definition

$$h_{\text{eff}}(\mathbf{k}) = \sum_{j=1}^m E_j(\mathbf{k}) |\Psi_j(\mathbf{k})\rangle \langle \Psi_j(\mathbf{k})|.$$

From the above we see that $h_{\text{eff}}(\mathbf{k})$ has $\Psi_j(\mathbf{k})$ as an eigenvector with corresponding eigenvalue $E_j(\mathbf{k})$.

Even though $h_{\text{eff}}(\mathbf{k})$ has a (redundant) constant zero eigenvalue, no information about the non-zero spectrum is lost. In particular, the m non-zero eigenvalues of the $M \times M$ matrix $h_{\text{eff}}(\mathbf{k})$, coinciding with the relevant Bloch bands, are periodic functions of \mathbf{k} and can be sampled at a few points \mathbf{k} in a mesh for $(-1/2, 1/2)^d$. Interpolating these few points with Fourier multipliers allows to approximate the energy bands with great accuracy: this is guaranteed by the smoothness of the constructed Parseval frame $\{\xi_a(\mathbf{k})\}$, which implies a very fast decay of their Fourier coefficients (namely of the corresponding Wannier functions) and hence a fast convergence of their Fourier series, see for example [116, 74] and references therein.

5.4 Non-periodic setting: results for irrational flux Hamiltonians

Once the construction of Parseval frames is established for periodic projections, it is a legitimate question to ask whether it is possible to extend this result to systems that are not periodic. Our second novel result goes in this direction. As was explained in Section 5.2, one such situation is provided by Hofstadter-like Hamiltonians on 2-dimensional crystals subject to a magnetic field which has irrational flux through the fundamental cell, in units of the magnetic flux quantum. As soon as the rationality condition is not satisfied, the Bloch bundle construction fails. This is due to the fact that, despite the Hamiltonian is still commuting with the set of magnetic translations, they are not a unitary representation of the translation group \mathbb{Z}^2 , but only a projective one. Therefore, since there is no \mathbf{k} -space description, one is forced to build spanning sets of localized vectors for the Fermi projection onto an isolated spectral island directly in position-space.

We approach the problem of an irrational magnetic flux perturbatively and set $b = b_0 + \epsilon$ with $b_0 q \in 2\pi\mathbb{Z}$ for $q \in \mathbb{N}$ and $0 \leq \epsilon \ll 1$. We assume that the periodic Hamiltonian $\tilde{\mathcal{H}}_0$ in (5.2.3), which is unitarily equivalent to the Hofstadter-like Hamiltonian H_{b_0} , has an isolated spectral island consisting of m bands which are associated to a Fermi projection $\tilde{\mathcal{P}}_0$ unitarily equivalent to the fibered operator $\int_{\mathbb{T}^2}^{\oplus} d\mathbf{k} P_0(\mathbf{k})$. Notice that, in the periodic Hamiltonian $\tilde{\mathcal{H}}_0$, the information about the magnetic field b_0 is encoded in the translation invariant matrix elements and the Peierls phase is absent, therefore $\tilde{\mathcal{H}}_0$ is a sort of effective reference non-magnetic Hamiltonian. If ϵ is small enough, then $\tilde{\mathcal{H}}_\epsilon$ will also have an isolated spectral island [29] associated to a Fermi projection $\tilde{\mathcal{P}}^{(\epsilon)}$, with $\tilde{\mathcal{P}}^{(\epsilon=0)} = \tilde{\mathcal{P}}_0$; notice that the number of magnetic mini-bands may change. Note that, as it was explained in Section 5.2, both $\tilde{\mathcal{H}}_\epsilon$ and $\tilde{\mathcal{P}}_\epsilon$ commute with the unitary operator defined in (5.2.10). Then our second main result is the following.

Theorem 5.4.1. *For $\eta \in \mathbb{Z}^2$, let $\tau_{\epsilon, \eta}$ be the unitary given defined in (5.2.10). Then there exists $\epsilon_0 > 0$ such that for all $0 \leq \epsilon \leq \epsilon_0$ the following hold:*

(i) there exist $m + 1$ exponentially localized vectors $\{w_a^{(\epsilon)}\}_{1 \leq a \leq m+1}$ such that

$$\tilde{\mathcal{P}}^{(\epsilon)} := \sum_{\eta \in \mathbb{Z}^2} \sum_{a=1}^{m+1} \left| \tau_{\epsilon, \eta} w_a^{(\epsilon)} \right\rangle \left\langle \tau_{\epsilon, \eta} w_a^{(\epsilon)} \right|; \quad (5.4.1)$$

(ii) if moreover $c_1(P_0) = 0 \in \mathbb{Z}$, where $c_1(P_0) \equiv c_1(P_0)_{12}$ is defined in (5.3.2), then there exist m exponentially localized vectors $\{w_a^{(\epsilon)}\}_{1 \leq a \leq m}$ such that the set $\{\tau_{\epsilon, \eta} w_a^{(\epsilon)}\}_{1 \leq a \leq m, \eta \in \mathbb{Z}^2}$ is an orthonormal basis of $\text{Ran } \tilde{\mathcal{P}}^{(\epsilon)}$.

In the same spirit of the proof of Theorem 5.3.2, our argument for the above result provides a constructive algorithm consisting of finitely many steps which exhibits the required Wannier functions.

The above result can be rephrased in terms of the original Hofstadter-like Hamiltonian $H_b = H_{b_0 + \epsilon}$. In order to do so, we refer to the notion, introduced in [82, 83] (see also [30]), of a generalized Wannier basis or Parseval frame for Hamiltonians which do not commute with a unitary representation of the group \mathbb{Z}^2 .

Definition 5.4.2. An exponentially localized generalized Wannier basis (respectively Parseval frame) for the projection Π acting in $\ell^2(\mathbb{Z}^2) \otimes \mathbb{C}^Q$ is a couple (Γ, \mathcal{W}) , where Γ is a discrete subset of \mathbb{R}^2 , and $\mathcal{W} = \{\psi_{\gamma, a}\}_{\gamma \in \Gamma, 1 \leq a \leq m(\gamma) < m^*}$, with $m^* > 0$ and independent of γ , is an orthonormal basis (respectively Parseval frame) for the range of Π such that

$$\sum_{\eta \in \mathbb{Z}^2} \sum_{x=1}^Q |\psi_{\gamma, a}(\eta, x)|^2 e^{\beta \|\eta - \gamma\|} \leq M, \quad a \in \{1, \dots, m(\gamma)\},$$

for some positive constants $\beta, M > 0$ uniform in γ .

Consider now the projection Π_b of the original Hofstadter-like Hamiltonian. As was explained in Section 5.2, at $b = b_0$ the Hamiltonian H_{b_0} is fibered by the magnetic Bloch–Floquet transform, $\mathcal{U}_{\text{mBF}} H_{b_0} \mathcal{U}_{\text{mBF}}^* = \int_{\mathbb{T}^2}^{\oplus} d\mathbf{k} h(\mathbf{k})$ (compare (5.2.8)), and correspondingly $\mathcal{U}_{\text{mBF}} \Pi_{b_0} \mathcal{U}_{\text{mBF}}^* = \int_{\mathbb{T}^2}^{\oplus} d\mathbf{k} P(\mathbf{k})$. Then the following result easily follows from Theorem 5.4.1 and Proposition 5.2.1.

Corollary 5.4.3. *There exists $\epsilon_0 > 0$ such that for all $0 \leq \epsilon \leq \epsilon_0$ the following hold:*

(i) there exists an exponentially localized generalized Wannier Parseval frame for the projection $\Pi_{b=b_0+\epsilon}$ that is given by the couple $(\mathbb{Z}^2, \{U_b^* \tau_{\epsilon, \eta} w_a^{(\epsilon)}\}_{\eta \in \mathbb{Z}^2, 1 \leq a \leq m+1})$ and satisfies

$$\Pi_b = \sum_{\eta \in \mathbb{Z}^2} \sum_{a=1}^{m+1} \left| U_b^* \tau_{\epsilon, \eta} w_a^{(\epsilon)} \right\rangle \left\langle U_b^* \tau_{\epsilon, \eta} w_a^{(\epsilon)} \right|.$$

(ii) if moreover $c_1(P) = 0 \in \mathbb{Z}$, where $c_1(P) \equiv c_1(P)_{12}$ is defined in (5.3.2), then there exists an exponentially localized generalized Wannier basis for the projection $\Pi_{b=b_0+\epsilon}$, given by $(\mathbb{Z}^2, \{U_b^* \tau_{\epsilon, \eta} w_a^{(\epsilon)}\}_{\eta \in \mathbb{Z}^2, 1 \leq a \leq m})$.

Let us stress that the unitary U_b consists just of multiplication by a local phase (compare (5.2.4)), hence it does not spoil the localization properties of the function on which it is applied.

The proofs of Theorem 5.4.1 and of its Corollary 5.4.3, crucially rely on Combes–Thomas estimates and on *gauge covariant magnetic perturbation theory* for discrete magnetic Hamiltonians, which we briefly review in Appendix A.2.5. These techniques are available also for continuous magnetic Schrödinger operators: see [37] and Appendix A.1 for the Combes–Thomas estimates, and [87, 29, 32] and Appendix 2.5.2 for magnetic perturbation theory. Thus, our proofs can be generalized to the continuous setting with only minor efforts (compare Remark 5.9.7).

The generalized Wannier Parseval frame $\{\psi_{\eta,a} := U_b^* \tau_{\epsilon,\eta} w_a^{(\epsilon)}\}_{\eta \in \mathbb{Z}^2, 1 \leq a \leq m}$ provided by Corollary 5.4.3 allows to construct effective Hamiltonians $h_{b,\text{eff}}(\eta, a; \eta', a') := \langle \psi_{\eta,a}, H_b \psi_{\eta',a'} \rangle$ on $\ell^2(\mathbb{Z}^2) \otimes \mathbb{C}^m$, from which spectral properties of the restriction to the isolated spectral island of the original Hofstadter-like Hamiltonian H_b can be investigated, compare Section 5.3.2 above.

Since we consider Corollary 5.4.3 as the most important and novel contribution of the chapter, we briefly sketch here the steps of its proof.

Step 1 First look at $b = b_0 \in 2\pi\mathbb{Q}$, or, said otherwise, at $\epsilon = 0$. The projection Π_0 is unitarily equivalent, via the modified Bloch–Floquet transform \mathcal{U}_{mBF} , to an analytic and \mathbb{Z}^2 -periodic family of rank- m projections $\{P(\mathbf{k})\}_{\mathbf{k} \in \mathbb{R}^2}$. Via a modified *parallel transport* in the second direction, one can extend any orthonormal basis for $P(\mathbf{0})$ to a smooth, \mathbb{Z} -periodic orthonormal Bloch basis for $\{P(0, k_2)\}_{k_2 \in \mathbb{R}}$. Again parallel transport in the first direction will lead to a smooth orthonormal Bloch basis $\{\psi_a(\mathbf{k})\}_{\mathbf{k} \in \mathbb{R}^2}$ for $\{P(\mathbf{k})\}_{\mathbf{k} \in \mathbb{R}^2}$, which fails however to be periodic in k_1 :

$$\psi_b(k_1 + 1, k_2) = \sum_{a=1}^m \psi_a(k_1, k_2) \alpha(k_2)_{ab}, \quad b \in \{1, \dots, m\}.$$

The unitary matrix $\alpha(k_2)$ is called the *matching matrix*.

Step 2 Via a *two-step logarithm*, the matching matrix can be deformed continuously to a diagonal matrix having all 1’s as the first $m - 1$ diagonal entries and a k_2 -dependent phase as the last entry. The latter can also be “unwinded”, that is, made equal to 1 for all $k_2 \in \mathbb{R}$, exactly when the Chern number of P vanishes. Deforming the matching matrix allows in turn to modify the ψ_a ’s to a new orthonormal Bloch basis where $m - 1$ vectors are also \mathbb{Z}^2 -periodic, while the last one picks up a (topological) phase when looping in the first direction over the Brillouin torus. A smoothing procedure further allows to choose this Bloch basis as a regular function of \mathbf{k} .

Step 3 Define $P_1(\mathbf{k})$ and $P_2(\mathbf{k})$ to be the subprojections of $P(\mathbf{k})$ onto the space spanned by the first $m - 1$ Bloch vectors constructed before and onto the orthogonal complement of their span, respectively. Then $\{P_2(\mathbf{k})\}_{\mathbf{k} \in \mathbb{R}^2}$ is a smooth and \mathbb{Z}^2 -periodic family of rank-1 projections. We *double the space dimension*, and consider the projection $P_2(\mathbf{k}) \oplus (CP_2(\mathbf{k})C^{-1})$, where C is a complex conjugation operator. This family of projections is topologically trivial and, by what was explained in Step 1, it admits a smooth and \mathbb{Z}^2 -periodic Bloch basis consisting of two vectors. By projecting these two Bloch vectors back to the original space, we obtain a Parseval 2-frame for

the rank-1 projection $P_2(\mathbf{k})$, and consequently also a Parseval $(m+1)$ -frame for $P(\mathbf{k})$, having all the desired properties.

Step 4 When applied to a rational-flux Hofstadter-like Hamiltonian H_{b_0} , the previous Steps produce an exponentially localized Wannier Parseval frame $\{\hat{\tau}_{b_0, \gamma} w_a\}_{1 \leq a \leq m, \gamma \in \mathbb{Z}^2}$ for Π_{b_0} by using the inverse magnetic Bloch–Floquet transform. We now perturb around b_0 , passing to $b = b_0 + \epsilon$. Recall from Proposition 5.2.1 that $H_{b_0+\epsilon} = U_{b_0+\epsilon}^* \tilde{\mathcal{H}}_\epsilon U_{b_0+\epsilon}$, where the matrix elements of $\tilde{\mathcal{H}}_\epsilon$ have the form (5.2.3). Inspired by gauge covariant magnetic perturbation theory [36, 87, 29], we consider the auxiliary Hamiltonian \mathcal{H}_ϵ defined through its matrix elements as in (5.2.3), but with the hopping \mathcal{T}_ϵ replaced by \mathcal{T}_0 . We prove that the spectra of $\tilde{\mathcal{H}}_\epsilon$ and of \mathcal{H}_ϵ are close (in the Hausdorff distance), and hence in particular that to every spectral projection $\tilde{\mathcal{P}}_\epsilon$ onto a gapped spectral island of $\tilde{\mathcal{H}}_\epsilon$ there corresponds a spectral projection \mathcal{P}_ϵ of \mathcal{H}_ϵ ; even more, for $|\epsilon|$ small enough the two projections are unitarily conjugated via a *Kato–Nagy unitary* K_ϵ . Thus a Wannier Parseval frame can be constructed for Π_b if and only if it can be constructed for \mathcal{P}_ϵ , since the two are unitarily conjugated via $U_{b_0+\epsilon} K_\epsilon$: the decay properties of the matrix elements of the latter unitary imply that localization is preserved under this unitary map.

Step 5 The projection \mathcal{P}_ϵ enjoys a number of properties, which we summarize in the Definition 5.8.2 of a *Fermi-like magnetic projection*. In particular, it is ϵ -close to the operator whose matrix elements are equal to the ones of \mathcal{P}_0 multiplied by the ϵ -dependent Peierls magnetic phase $e^{i\epsilon\phi(\cdot)}$. The latter is not a projection anymore (it squares to itself only up to errors of order ϵ), but it is much better-behaved as a function of ϵ . Exploiting gauge covariant magnetic perturbation theory coupled with the procedure in Step 3, we find localized vectors close to the magnetic translates via $\tau_{\epsilon, \gamma}$ of the ones constructed previously at $\epsilon = 0$, which give the required Parseval frame for \mathcal{P}_ϵ (and hence for Π_b by Step 4). See the discussion after Proposition 5.9.1 for a more detailed description of this procedure.

5.5 Proof of Theorem 5.3.2(iii): the topologically trivial case

We begin by proving Theorem 5.3.2(iii) since elements of this proof will be essential for the other two parts of Theorem 5.3.2. Thus we assume throughout this section that $\{P(\mathbf{k})\}_{\mathbf{k} \in \mathbb{R}^d}$, $d \leq 3$, is a smooth and \mathbb{Z}^d -periodic family of rank- m projections on the Hilbert space \mathcal{H} with vanishing Chern numbers. We will construct an orthonormal Bloch basis (so, a m -tuple of orthogonal Bloch vectors) which is continuous and \mathbb{Z}^d -periodic. To stress that our proofs are algorithmic and explicit in nature, we use the phrase “one can construct...” in many of the following statements.

5.5.1 The 1D case

We start from the case $d = 1$. Notice that any 1-dimensional family of projections $\{P(k)\}_{k \in \mathbb{R}}$ is topologically trivial, that is, it has vanishing Chern numbers (as there are no non-zero differential 2-forms on the circle \mathbb{T}).

Let $T(k, 0)$ denote the parallel transport unitary along the segment from the point 0 to the point k associated to $\{P(k)\}_{k \in \mathbb{R}}$ (see Appendix A.2.2 for more details). At $k = 1$, write $T(1, 0) = e^{iM}$, where $M = M^* \in \mathcal{B}(\mathcal{H})$ is self-adjoint.

Pick an orthonormal basis $\{\xi_a(0)\}_{a=1}^m$ in $\text{Ran } P(0) \simeq \mathbb{C}^m \subset \mathcal{H}$, and define for $a \in \{1, \dots, m\}$ and $k \in \mathbb{R}$

$$\xi_a(k) := W(k) \xi_a(0), \quad W(k) := T(k, 0)e^{-ikM}.$$

Then $\{\xi_a\}_{a=1}^m$ gives a continuous, \mathbb{Z}^2 -periodic, and orthonormal Bloch basis for the 1-dimensional family of projections $\{P(k)\}_{k \in \mathbb{R}}$ (compare [30, 34]). This proves Theorem 5.3.2 in $d = 1$ (where the only non-trivial statement is part (iii)).

5.5.2 The induction argument in the dimension

Consider a smooth and periodic family of projections $\{P(k_1, \mathbf{k})\}_{(k_1, \mathbf{k}) \in \mathbb{R}^d}$, and let $D := d - 1$. Assume that the D -dimensional restriction $\{P(0, \mathbf{k})\}_{\mathbf{k} \in \mathbb{R}^D}$ admits a continuous and \mathbb{Z}^D -periodic orthonormal Bloch basis $\{\xi_a(0, \cdot)\}_{a=1}^m$. Consider now the parallel transport unitary $T_{\mathbf{k}}(k_1, 0)$ along the straight line from the point $(0, \mathbf{k})$ to the point (k_1, \mathbf{k}) . At $k_1 = 1$, denote $\mathcal{T}(\mathbf{k}) := T_{\mathbf{k}}(1, 0)$. Define

$$\psi_a(k_1, \mathbf{k}) := T_{\mathbf{k}}(k_1, 0) \xi_a(0, \mathbf{k}), \quad a \in \{1, \dots, m\}, \quad (k_1, \mathbf{k}) \in \mathbb{R}^d. \quad (5.5.1)$$

The above defines a collection of m Bloch vectors for $\{P(k_1, \mathbf{k})\}_{(k_1, \mathbf{k}) \in \mathbb{R}^d}$ which are continuous, orthonormal, and \mathbb{Z}^D -periodic in the variable \mathbf{k} , but in general fail to be \mathbb{Z} -periodic in the variable k_1 . Indeed, one can check that

$$\psi_b(k_1 + 1, \mathbf{k}) = \sum_{a=1}^m \psi_a(k_1, \mathbf{k}) \alpha(\mathbf{k})_{ab}, \quad \text{where } \alpha(\mathbf{k})_{ab} := \langle \xi_a(0, \mathbf{k}), \mathcal{T}(\mathbf{k}) \xi_b(0, \mathbf{k}) \rangle \quad (5.5.2)$$

(compare [34, Eqn.s (3.4) and (3.5)]). The family $\{\alpha(\mathbf{k})\}_{\mathbf{k} \in \mathbb{R}^D}$ defined above is a continuous and \mathbb{Z}^D -periodic family of $m \times m$ unitary matrices.

The possibility of “rotating” $\alpha(\mathbf{k})$ to the identity entails thus the construction of a Bloch basis which is also periodic in k_1 . Formally, we have the following statement (compare also [31, Thm.s 2.4 and 2.6]).

Proposition 5.5.1. *For the continuous and periodic family $\{\alpha(\mathbf{k})\}_{\mathbf{k} \in \mathbb{R}^D}$ defined in (5.5.2), the following are equivalent:*

- (i) *the family is null-homotopic, namely there exists a collection of continuous and \mathbb{Z}^D -periodic family of unitary matrices $\{\alpha_t(\mathbf{k})\}_{\mathbf{k} \in \mathbb{R}^D}$, depending continuously on $t \in [0, 1]$, and such that $\alpha_{t=0}(\mathbf{k}) \equiv \mathbf{1}$ while $\alpha_{t=1}(\mathbf{k}) = \alpha(\mathbf{k})$ for all $\mathbf{k} \in \mathbb{R}^D$;*
- (ii) *assuming $D \leq 2$, we have $\deg_j(\det \alpha) = 0$ for all $j \in \{1, \dots, D\}$. In the smooth case, this is the same as:*

$$\deg_j(\det \alpha) = \frac{1}{2\pi i} \int_0^1 dk_j \text{tr}_{\mathbb{C}^m} \left(\alpha(\mathbf{k})^* \frac{\partial \alpha}{\partial k_j}(\mathbf{k}) \right) = 0 \quad \text{for all } j \in \{1, \dots, D\}; \quad (5.5.3)$$

(iii) the family admits a continuous and \mathbb{Z}^D -periodic N -step logarithm, namely there exist N continuous and \mathbb{Z}^D -periodic families of self-adjoint matrices $\{h_i(\mathbf{k})\}_{\mathbf{k} \in \mathbb{R}^D}$, $i \in \{1, \dots, N\}$, such that

$$\alpha(\mathbf{k}) = e^{ih_1(\mathbf{k})} \dots e^{ih_N(\mathbf{k})}, \quad \mathbf{k} \in \mathbb{R}^D; \quad (5.5.4)$$

(iv) there exists a continuous family of unitary matrices $\{\beta(k_1, \mathbf{k})\}_{(k_1, \mathbf{k}) \in \mathbb{R}^d}$, $d = D + 1$, which is \mathbb{Z}^D -periodic in \mathbf{k} , with $\beta(0, \mathbf{k}) \equiv \mathbf{1}$ for all $\mathbf{k} \in \mathbb{R}^D$, and such that

$$\alpha(\mathbf{k}) = \beta(k_1, \mathbf{k}) \beta(k_1 + 1, \mathbf{k})^{-1}, \quad (k_1, \mathbf{k}) \in \mathbb{R}^d;$$

(v) there exists a continuous and \mathbb{Z}^d -periodic Bloch basis $\{\xi_a\}_{a=1}^m$ for $\{P(\mathbf{k})\}_{\mathbf{k} \in \mathbb{R}^d}$.

Proof. (i) \iff (ii). The integer $\deg_j(\det \alpha)$ defined in (5.5.3) computes the winding number of the continuous and periodic function $k_j \mapsto \det \alpha(\dots, k_j, \dots): \mathbb{R} \rightarrow U(1)$, $j \in \{1, \dots, D\}$. It is a well-known fact in topology that $\pi_1(U(m)) \simeq \pi_1(U(1)) \simeq \mathbb{Z}$, with the first isomorphism implemented by the map $[\alpha] \mapsto [\det \alpha]$ and the second one implemented by the map $[\varphi] \mapsto \deg(\varphi) := (2\pi i)^{-1} \int_0^1 \varphi^{-1} d\varphi$. It can be then argued that these winding numbers constitute complete homotopy invariants for continuous, periodic maps $\alpha: \mathbb{R}^D \rightarrow U(m)$ when $D \leq 2$ (see e.g [80, App. A]).

(i) \iff (iii). Let $\{\alpha_t(\mathbf{k})\}_{\mathbf{k} \in \mathbb{R}^D}$ be an homotopy between $\mathbf{1}$ and α , as in the statement. Since $[0, 1]$ is a compact interval and α_t is \mathbb{Z}^D -periodic, by uniform continuity there exists $\delta > 0$ such that

$$\sup_{\mathbf{k} \in \mathbb{R}^D} \|\alpha_s(\mathbf{k}) - \alpha_t(\mathbf{k})\| < 2 \quad \text{whenever} \quad |s - t| < \delta. \quad (5.5.5)$$

Let $N \in \mathbb{N}$ be such that $1/N < \delta$. Then in particular

$$\sup_{\mathbf{k} \in \mathbb{R}^D} \|\alpha_{1/N}(\mathbf{k}) - \mathbf{1}\| < 2$$

so that the Cayley transform (see Appendix A.2.3) provides a “good” logarithm for $\alpha_{1/N}(\mathbf{k})$, i.e. $\alpha_{1/N}(\mathbf{k}) = e^{ih_N(\mathbf{k})}$, with $h_N(\mathbf{k}) = h_N(\mathbf{k})^*$ continuous and \mathbb{Z}^D -periodic.

Using again (5.5.5) we have that

$$\sup_{\mathbf{k} \in \mathbb{R}^D} \|\alpha_{2/N}(\mathbf{k}) e^{-ih_N(\mathbf{k})} - \mathbf{1}\| = \sup_{\mathbf{k} \in \mathbb{R}^D} \|\alpha_{2/N}(\mathbf{k}) - \alpha_{1/N}(\mathbf{k})\| < 2$$

so that by the same argument

$$\alpha_{2/N}(\mathbf{k}) e^{-ih_N(\mathbf{k})} = e^{ih_{N-1}(\mathbf{k})}, \quad \text{or} \quad \alpha_{2/N}(\mathbf{k}) = e^{ih_{N-1}(\mathbf{k})} e^{ih_N(\mathbf{k})}.$$

Repeating the same line of reasoning N times, we end up exactly with (5.5.4).

Conversely, if $\alpha(\mathbf{k})$ is as in (5.5.4), then

$$\alpha_t(\mathbf{k}) := e^{ith_1(\mathbf{k})} \dots e^{ith_N(\mathbf{k})}, \quad t \in [0, 1], \quad \mathbf{k} \in \mathbb{R}^D,$$

defines the required homotopy between $\alpha_0(\mathbf{k}) \equiv \mathbf{1}$ and $\alpha_1(\mathbf{k}) = \alpha(\mathbf{k})$.

(i) \iff (iv). Let $\{\alpha_t(\mathbf{k})\}_{\mathbf{k} \in \mathbb{R}^D}$ be an homotopy between $\mathbf{1}$ and α . We set

$$\beta(k_1, \mathbf{k}) := \alpha_{k_1}(\mathbf{k})^{-1}, \quad k_1 \in [0, 1], \quad \mathbf{k} \in \mathbb{R}^D,$$

and extend this definition to positive $k_1 > 0$ via

$$\beta(k_1 + 1, \mathbf{k}) := \alpha(\mathbf{k})^{-1} \beta(k_1, \mathbf{k})$$

and to negative $k_1 < 0$ via

$$\beta(k_1, \mathbf{k}) := \alpha(\mathbf{k}) \beta(k_1 + 1, \mathbf{k}).$$

We just need to show that this definition yields a continuous function of k_1 . We have $\beta(0^+, \mathbf{k}) = \mathbf{1}$ and $\beta(1^-, \mathbf{k}) = \alpha(\mathbf{k})^{-1}$ by definition. Let $\epsilon > 0$. If $k_1 = -\epsilon$ is negative but close to zero, we have due to the definition

$$\beta(-\epsilon, \mathbf{k}) = \alpha(\mathbf{k}) \beta(1 - \epsilon, \mathbf{k}) \rightarrow \alpha(\mathbf{k}) \beta(1^-, \mathbf{k}) = \mathbf{1} \quad \text{as } \epsilon \rightarrow 0.$$

Hence β is continuous at $k_1 = 0$. At $k_1 = 1$ we have instead

$$\beta(1 + \epsilon, \mathbf{k}) = \alpha(\mathbf{k})^{-1} \beta(\epsilon, \mathbf{k}) \rightarrow \alpha(\mathbf{k})^{-1} \beta(0^+, \mathbf{k}) = \alpha(\mathbf{k})^{-1} \quad \text{as } \epsilon \rightarrow 0$$

and β is also continuous there. In a similar way one can prove continuity at every integer, thus on \mathbb{R} .

Conversely, if $\{\beta(k_1, \mathbf{k})\}_{(k_1, \mathbf{k}) \in \mathbb{R}^2}$ is as in the statement, then the required homotopy α_t between $\mathbf{1}$ and α is provided by setting

$$\alpha_t(\mathbf{k}) := \beta(-t/2, \mathbf{k}) \beta(t/2, \mathbf{k})^{-1}, \quad t \in [0, 1], \quad \mathbf{k} \in \mathbb{R}^D.$$

(iv) \iff (v). It suffices to set

$$\xi_a(k_1, \mathbf{k}) := \sum_{b=1}^m \psi_b(k_1, \mathbf{k}) \beta(k_1, \mathbf{k})_{ba}, \quad a \in \{1, \dots, m\},$$

or equivalently

$$\beta(k_1, \mathbf{k})_{ba} := \langle \psi_b(k_1, \mathbf{k}), \xi_a(k_1, \mathbf{k}) \rangle, \quad a, b \in \{1, \dots, m\},$$

for $\{\psi_b\}_{b=1}^m$ as in (5.5.1) and $(k_1, \mathbf{k}) \in \mathbb{R}^d$. \square

To turn the above proof into a constructive argument, we need to construct the “good” logarithms in (5.5.4).

Proposition 5.5.2. *For $D \leq 2$, let $\{\alpha(\mathbf{k})\}_{\mathbf{k} \in \mathbb{R}^D}$ be a continuous and \mathbb{Z}^D -periodic family of unitary matrices. Assume that α is null-homotopic. Then it is possible to construct a two-step “good” logarithm for α , i.e. $N = 2$ in Proposition 5.5.1(iii).*

Proof. Step 1 : the generic form. We first need to know that one can construct a sequence of continuous, \mathbb{Z}^D -periodic families of unitary matrices $\{\alpha_n(\mathbf{k})\}_{\mathbf{k} \in \mathbb{R}^D}$, $n \in \mathbb{N}$, such that

- $\sup_{\mathbf{k} \in \mathbb{R}^D} \|\alpha_n(\mathbf{k}) - \alpha(\mathbf{k})\| \rightarrow 0$ as $n \rightarrow \infty$, and

- the spectrum of $\alpha_n(\mathbf{k})$ is completely non-degenerate for all $n \in \mathbb{N}$ and $\mathbf{k} \in \mathbb{R}^D$.

The proof of this fact is rather technical, and is deferred to Appendix A.2.4. In the following, we denote $\alpha'(\mathbf{k}) := \alpha_n(\mathbf{k})$ where $n \in \mathbb{N}$ is large enough so that

$$\sup_{\mathbf{k} \in \mathbb{R}^D} \|\alpha'(\mathbf{k}) - \alpha(\mathbf{k})\| < 2.$$

Step 2 : α' is homotopic to α . Since

$$\sup_{\mathbf{k} \in \mathbb{R}^D} \left\| \alpha'(\mathbf{k}) \alpha(\mathbf{k})^{-1} - \mathbf{1} \right\| = \sup_{\mathbf{k} \in \mathbb{R}^D} \|\alpha'(\mathbf{k}) - \alpha(\mathbf{k})\| < 2$$

we have that -1 always lies in the resolvent set of $\alpha'(\mathbf{k}) \alpha(\mathbf{k})^{-1}$, which then admits a continuous and \mathbb{Z}^D -periodic logarithm defined via the Cayley transform:

$$\alpha'(\mathbf{k}) \alpha(\mathbf{k})^{-1} = e^{ih''(\mathbf{k})}, \quad h''(\mathbf{k})^* = h''(\mathbf{k}) = h''(\mathbf{k} + \mathbf{n}) \text{ for } \mathbf{n} \in \mathbb{Z}^D. \quad (5.5.6)$$

Therefore

$$\alpha_t(\mathbf{k}) := \alpha'(\mathbf{k}) e^{it h''(\mathbf{k})}, \quad t \in [0, 1], \quad \mathbf{k} \in \mathbb{R}^D,$$

gives a continuous homotopy between $\alpha_0(\mathbf{k}) = \alpha'(\mathbf{k})$ and $\alpha_1(\mathbf{k}) = \alpha(\mathbf{k})$. As a consequence, we have that α' is null-homotopic, since α is by assumption.

Step 3 : a logarithm for α' . Denote by $\{\lambda_1(\mathbf{k}), \dots, \lambda_m(\mathbf{k})\}$ a continuous labelling of the periodic, non-degenerate eigenvalues of $\alpha'(\mathbf{k})$.

If $m = 1$, then $\alpha'(\mathbf{k}) \equiv \det(\alpha'(\mathbf{k})) \equiv \lambda_1(\mathbf{k})$ cannot wind around the circle, due to the hypothesis that α' is null-homotopic. This implies that one can choose a continuous and *periodic* argument for λ_1 , namely $\lambda_1(\mathbf{k}) = e^{i\phi_1(\mathbf{k})}$ with $\phi_1: \mathbb{R}^D \rightarrow \mathbb{R}$ continuous and \mathbb{Z}^D -periodic (compare e.g. [30, Lemma 2.13]).

If $m \geq 2$, then the same is true for each of the eigenvalues $\lambda_j(\mathbf{k})$, $j \in \{1, \dots, m\}$. Indeed, let $\phi_j: \mathbb{R}^D \rightarrow \mathbb{R}$ be a continuous argument of the eigenvalue λ_j . The function ϕ_j will satisfy

$$\phi_j(\mathbf{k} + \mathbf{e}_l) = \phi_j(\mathbf{k}) + 2\pi n_j^{(l)}, \quad l \in \{1, \dots, D\}, \quad n_j^{(l)} \in \mathbb{Z},$$

where $\mathbf{e}_l = (0, \dots, 1, \dots, 0)$ is the l -th vector in the standard basis of \mathbb{R}^D and the integer $n_j^{(l)}$ is the winding number of the periodic function $\mathbb{R} \rightarrow U(1)$, $k_l \mapsto \lambda_j(\dots, k_l, \dots)$. Fix $l \in \{1, \dots, D\}$, and assume that there exist $i, j \in \{1, \dots, m\}$ for which $n_i^{(l)} \neq n_j^{(l)}$. Define $\phi(\mathbf{k}) := \phi_j(\mathbf{k}) - \phi_i(\mathbf{k})$; then

$$\phi(\mathbf{k} + \mathbf{e}_l) = \phi(\mathbf{k}) + 2\pi (n_j^{(l)} - n_i^{(l)}).$$

Since $n_j^{(l)} - n_i^{(l)} \neq 0$, the periodic function $\lambda(\mathbf{k}) := e^{i\phi(\mathbf{k})}$ winds around the circle $U(1)$ at least once as a function of the l -th component, and in particular covers the whole circle. So there must exist $\mathbf{k}_0 \in \mathbb{R}^D$ such that $\lambda(\mathbf{k}_0) = 1$, or equivalently $\lambda_i(\mathbf{k}_0) = e^{i\phi_i(\mathbf{k}_0)} = e^{i\phi_j(\mathbf{k}_0)} = \lambda_j(\mathbf{k}_0)$, in contradiction with the non-degeneracy of the eigenvalues of $\alpha'(\mathbf{k})$.

We deduce then that $n_i^{(l)} = n_j^{(l)} \equiv n^{(l)}$ for all $i, j \in \{1, \dots, m\}$. Set now $\det(\alpha'(\mathbf{k})) = e^{i\Phi(\mathbf{k})}$ for $\Phi(\mathbf{k}) = \phi_1(\mathbf{k}) + \dots + \phi_m(\mathbf{k})$. Then the equality

$$\Phi(\mathbf{k} + \mathbf{e}_l) = \Phi(\mathbf{k}) + 2\pi \sum_{j=1}^m n_j^{(l)} = \Phi(\mathbf{k}) + 2\pi m n^{(l)}$$

shows that necessarily $n^{(l)} = 0$ for all $l \in \{1, \dots, D\}$, as otherwise the determinant of α' would wind around the circle contrary to the hypothesis of null-homotopy of α' .

Finally, denote by $0 < g \leq 2$ the minimal distance between any two eigenvalues of $\alpha'(\mathbf{k})$, and define the continuous and periodic function $\rho(\mathbf{k}) := \phi_1(\mathbf{k}) + g/100$. Then $e^{i\rho(\mathbf{k})}$ lies in the resolvent set of $\alpha'(\mathbf{k})$ for all $\mathbf{k} \in \mathbb{R}$. As a consequence, -1 is always in the resolvent set of the continuous and periodic family of unitary matrices $\tilde{\alpha}(\mathbf{k}) := e^{-i(\rho(\mathbf{k})+\pi)} \alpha'(\mathbf{k})$, which then admits a continuous and periodic logarithm via the Cayley transform: $\tilde{\alpha}(\mathbf{k}) = e^{i\tilde{h}(\mathbf{k})}$. We conclude that

$$\alpha'(\mathbf{k}) = e^{ih'(\mathbf{k})} \quad \text{with} \quad h'(\mathbf{k}) := \tilde{h}(\mathbf{k}) + (\rho(\mathbf{k}) + \pi)\mathbf{1}. \quad (5.5.7)$$

The family of self-adjoint matrices $\{h'(\mathbf{k})\}_{\mathbf{k} \in \mathbb{R}^D}$ is still continuous and periodic by definition.

Step 4 : a two-step logarithm for α . In view of (5.5.6) and (5.5.7) we have $e^{ih'(\mathbf{k})} \alpha(\mathbf{k})^{-1} = e^{ih''(\mathbf{k})}$ for continuous and periodic families of self-adjoint matrices $\{h'(\mathbf{k})\}_{\mathbf{k} \in \mathbb{R}^D}$ and $\{h''(\mathbf{k})\}_{\mathbf{k} \in \mathbb{R}^D}$. This can be rewritten as $\alpha(\mathbf{k}) = e^{-ih''(\mathbf{k})} e^{ih'(\mathbf{k})}$, which is (5.5.4) for $N = 2$. \square

5.5.3 The link between the topology of α and that of P

We now come back to Theorem 5.3.2(iii). First we consider the case $d = 2$ (so that $D = d - 1 = 1$). We have constructed in (5.5.2) a continuous and \mathbb{Z} -periodic family of unitary matrices $\{\alpha(k_2)\}_{k_2 \in \mathbb{R}}$, starting from a smooth, periodic family of projections $\{P(k_1, k_2)\}_{(k_1, k_2) \in \mathbb{R}^2}$ and an orthonormal Bloch basis for the restriction $\{P(0, k_2)\}_{k_2 \in \mathbb{R}}$. The next result links the topology of α with the one of P .

Proposition 5.5.3. *Let $\{\alpha(k_2)\}_{k_2 \in \mathbb{R}}$ and $\{P(\mathbf{k})\}_{\mathbf{k} \in \mathbb{R}^2}$ be as above. Then*

$$\deg(\det \alpha) = c_1(P).$$

Proof. The equality in the statement follows at once from the following chain of equalities:

$$\begin{aligned} \text{tr}_{\mathcal{C}^m} (\alpha(k_2)^* \partial_{k_2} \alpha(k_2)) &= \text{Tr}_{\mathcal{H}} (P(0, k_2) \mathcal{T}(k_2)^* \partial_{k_2} \mathcal{T}(k_2)) \\ &= \int_0^1 dk_1 \text{Tr}_{\mathcal{H}} (P(\mathbf{k}) [\partial_1 P(\mathbf{k}), \partial_2 P(\mathbf{k})]). \end{aligned}$$

Their proof can be found in Appendix A.2.2 (compare [34, Sec. 6.3]). \square

We are finally able to conclude the proof of Theorem 5.3.2(iii).

Proof of Theorem 5.3.2(iii), $d = 2$. Given our initial hypothesis that $c_1(P) = 0$, the combination of Propositions 5.5.1 and 5.5.3 gives that α is null-homotopic, and hence admits a two-step logarithm which can be constructed via Proposition 5.5.2. This construction then yields the desired continuous and periodic Bloch basis, again via Proposition 5.5.1. \square

Proof of Theorem 5.3.2(iii), $d = 3$. Let $\{P(k_1, k_2, k_3)\}_{(k_1, k_2, k_3) \in \mathbb{R}^3}$ be a smooth and periodic family of projections. Under the assumption that $c_1(P)_{23} = 0$, the 2-dimensional result we just proved provides an orthonormal Bloch basis for the restriction $\{P(0, k_2, k_3)\}_{(k_2, k_3) \in \mathbb{R}^2}$, which can be parallel-transported to $\{k_1 = 1\}$ and hence defines $\{\alpha(k_2, k_3)\}_{(k_2, k_3) \in \mathbb{R}^2}$, as in (5.5.2). We now apply Proposition 5.5.3, to the 2-dimensional restrictions $\{P(k_1, 0, k_3)\}_{(k_1, k_3) \in \mathbb{R}^2}$ and $\{P(k_1, k_2, 0)\}_{(k_1, k_2) \in \mathbb{R}^2}$ instead, and obtain that

$$\begin{aligned} \deg_2(\det \alpha) &= \deg(\det \alpha(\cdot, 0)) = c_1(P)_{12} = 0, \\ \deg_3(\det \alpha) &= \deg(\det \alpha(0, \cdot)) = c_1(P)_{13} = 0 \end{aligned} \tag{5.5.8}$$

(compare Appendix A.2.2). Again by Proposition 5.5.1 the family α is then null-homotopic, and one can construct its two-step logarithm via Proposition 5.5.2. Proposition 5.5.1 illustrates how to produce the required continuous and \mathbb{Z}^3 -periodic Bloch basis. \square

5.6 Proof of Theorem 5.3.2(i): maximal number of orthonormal Bloch vectors

We come to the proof of Theorem 5.3.2(i), concerning the existence of $m - 1$ orthonormal Bloch vectors for a smooth and \mathbb{Z}^d -periodic family of projections $\{P(\mathbf{k})\}_{\mathbf{k} \in \mathbb{R}^d}$ with $2 \leq d \leq 3$. As usual, we have denoted by m the rank of $P(\mathbf{k})$.

5.6.1 Pseudo-periodic families of matrices

Before giving the proof of Theorem 5.3.2(i), we need some generalizations of the results in Section 5.5.2.

Definition 5.6.1. Let $\{\gamma(k_3)\}_{k_3 \in \mathbb{R}}$ be a continuous and \mathbb{Z} -periodic family of unitary matrices. We say that a continuous family of matrices $\{\mu(k_2, k_3)\}_{(k_2, k_3) \in \mathbb{R}^2}$ is γ -periodic if it satisfies the following conditions:

$$\mu(k_2 + 1, k_3) = \gamma(k_3) \mu(k_2, k_3) \gamma(k_3)^{-1}, \quad \mu(k_2, k_3 + 1) = \mu(k_2, k_3), \quad (k_2, k_3) \in \mathbb{R}^2.$$

We say that two continuous and γ -periodic families $\{\mu_0(\mathbf{k})\}_{\mathbf{k} \in \mathbb{R}^2}$ and $\{\mu_1(\mathbf{k})\}_{\mathbf{k} \in \mathbb{R}^2}$ are γ -homotopic if there exists a collection of continuous and γ -periodic families $\{\mu_t(\mathbf{k})\}_{\mathbf{k} \in \mathbb{R}^2}$, depending continuously on $t \in [0, 1]$, such that $\mu_{t=0}(\mathbf{k}) = \mu_0(\mathbf{k})$ and $\mu_{t=1}(\mathbf{k}) = \mu_1(\mathbf{k})$ for all $\mathbf{k} \in \mathbb{R}^2$.

Notice that a γ -periodic family of matrices is periodic in k_3 and only pseudo-periodic in k_2 : the family γ encodes the failure of k_2 -periodicity.

Proposition 5.6.2. *Let $\{\alpha(k_2, k_3)\}_{(k_2, k_3) \in \mathbb{R}^2}$ be a continuous and γ -periodic family of unitary matrices, and assume that $\deg_2(\det \alpha) = \deg_3(\det \alpha) = 0$. Then one can construct a continuous and γ -periodic two-step logarithm for α , namely there exist continuous and γ -periodic families of self-adjoint matrices $\{h_i(\mathbf{k})\}_{\mathbf{k} \in \mathbb{R}^2}$, $i \in \{1, 2\}$, such that*

$$\alpha(k_2, k_3) = e^{ih_1(k_2, k_3)} e^{ih_2(k_2, k_3)}, \quad (k_2, k_3) \in \mathbb{R}^2.$$

Proof. The argument goes as in the proof of Proposition 5.5.2. One just needs to modify Step 1 there, where the approximants of α with completely non-degenerate spectrum are constructed obeying γ -periodicity rather than mere periodicity (compare Appendix A.2.4). It is also worth noting that both the spectrum and the norm of $\mu(k_2 + 1, k_3)$ coincide with the spectrum and the norm of $\mu(k_2, k_3)$ for any γ -periodic family of matrices μ , and that the Cayley transform of a γ -periodic family of unitary matrices $\{\alpha(k_2, k_3)\}_{(k_2, k_3) \in \mathbb{R}^2}$ is also γ -periodic. Hence, logarithms constructed via functional calculus on the Cayley transform are automatically γ -periodic (see Appendix A.2.3). Finally, observing that the spectrum of a γ -periodic family of matrices is \mathbb{Z}^2 -periodic, the rest of the argument for Proposition 5.5.2 goes through unchanged. \square

The next result generalizes Proposition 5.5.1 considerably.

Proposition 5.6.3. *Assume that $D \leq 2$. Let $\{\alpha_0(\mathbf{k})\}_{\mathbf{k} \in \mathbb{R}^D}$ and $\{\alpha_1(\mathbf{k})\}_{\mathbf{k} \in \mathbb{R}^D}$ be continuous and periodic families of unitary matrices. Then the following are equivalent:*

- (i) *the families are homotopic;*
- (ii) *$\deg_j(\det \alpha_0) = \deg_j(\det \alpha_1)$ for all $j \in \{1, \dots, D\}$, where $\deg_j(\det \cdot)$ is defined in (5.5.3);*
- (iii) *one can construct a continuous family of unitary matrices $\{\beta(k_1, \mathbf{k})\}_{(k_1, \mathbf{k}) \in \mathbb{R}^d}$, $d = D + 1$, which is \mathbb{Z}^D -periodic in \mathbf{k} , with $\beta(0, \mathbf{k}) \equiv \mathbf{1}$ for all $\mathbf{k} \in \mathbb{R}^D$, and such that*

$$\alpha_1(\mathbf{k}) = \beta(k_1, \mathbf{k}) \alpha_0(\mathbf{k}) \beta(k_1 + 1, \mathbf{k})^{-1}, \quad (k_1, \mathbf{k}) \in \mathbb{R}^d.$$

If $D = 2$, then the above three statements remain equivalent even if one replaces periodicity by γ -periodicity and homotopy by γ -homotopy.

Proof. Since periodicity is a particular case of γ -periodicity, we give the proof in the γ -periodic framework. Set

$$\alpha'(\mathbf{k}) := \alpha_1(\mathbf{k})^{-1} \alpha_0(\mathbf{k}), \quad \mathbf{k} \in \mathbb{R}^D.$$

Then $\{\alpha'(\mathbf{k})\}_{\mathbf{k} \in \mathbb{R}^D}$ is a continuous and γ -periodic family of unitary matrices, satisfying moreover $\deg_j(\det \alpha') = \deg_j(\det \alpha_0) - \deg_j(\det \alpha_1) = 0$ for $j \in \{1, \dots, D\}$. In view of Proposition 5.6.2, one can construct a continuous and γ -periodic two-step logarithm for α' :

$$\alpha'(\mathbf{k}) = e^{ih_2(\mathbf{k})} e^{ih_1(\mathbf{k})}.$$

Define

$$\beta(k_1, \mathbf{k}) := e^{ik_1 h_2(\mathbf{k})} e^{ik_1 h_1(\mathbf{k})}, \quad k_1 \in [0, 1], \mathbf{k} \in \mathbb{R}^D,$$

and extend this definition to positive $k_1 > 0$ by

$$\beta(k_1 + 1, \mathbf{k}) := \alpha_1(\mathbf{k})^{-1} \beta(k_1, \mathbf{k}) \alpha_0(\mathbf{k})$$

and to negative $k_1 < 0$ by

$$\beta(k_1, \mathbf{k}) := \alpha_1(\mathbf{k}) \beta(k_1 + 1, \mathbf{k}) \alpha_0(\mathbf{k})^{-1}.$$

Notice first that the above defines a family of unitary matrices which is γ -periodic in \mathbf{k} . We just need to show that this definition yields also a continuous function of k_1 . We have $\beta(0^+, \mathbf{k}) = \mathbf{1}$ and $\beta(1^-, k_2) = \alpha_1(\mathbf{k})^{-1} \alpha_0(\mathbf{k})$ by definition. Let $\epsilon > 0$. If $k_1 = -\epsilon$ is negative but close to zero, we have due to the definition

$$\beta(-\epsilon, \mathbf{k}) = \alpha_1(\mathbf{k}) \beta(1 - \epsilon, \mathbf{k}) \alpha_0(\mathbf{k})^{-1} \rightarrow \alpha_1(\mathbf{k}) \beta(1^-, \mathbf{k}) \alpha_0(\mathbf{k})^{-1} = \mathbf{1} \quad \text{as } \epsilon \rightarrow 0.$$

Hence β is continuous at $k_1 = 0$. At $k_1 = 1$ we have instead

$$\beta(1 + \epsilon, \mathbf{k}) = \alpha_1(\mathbf{k})^{-1} \beta(\epsilon, \mathbf{k}) \alpha_0(\mathbf{k}) \rightarrow \alpha_1(\mathbf{k})^{-1} \beta(0^+, \mathbf{k}) \alpha_0(\mathbf{k}) = \alpha_1(\mathbf{k})^{-1} \alpha_0(\mathbf{k})$$

as $\epsilon \rightarrow 0$, and β is also continuous there. A similar argument shows continuity of $k_1 \mapsto \beta(k_1, \mathbf{k})$ at every other integer value of k_1 .

Conversely, if we are given $\{\beta(k_1, \mathbf{k})\}_{(k_1, \mathbf{k}) \in \mathbb{R}^3}$ as in the statement, then

$$\alpha_t(\mathbf{k}) := \beta(-t/2, \mathbf{k}) \alpha_0(\mathbf{k}) \beta(t/2, \mathbf{k})^{-1}, \quad t \in [0, 1], \mathbf{k} \in \mathbb{R}^2,$$

gives the desired γ -homotopy between α_0 and α_1 . □

5.6.2 Orthonormal Bloch vectors

We now come back to the proof of Theorem 5.3.2(i).

Proof of Theorem 5.3.2(i). Let us start from a 2-dimensional smooth and \mathbb{Z}^2 -periodic family of rank- m projections $\{P(\mathbf{k})\}_{\mathbf{k} \in \mathbb{R}^2}$. We replicate the construction at the beginning of Section 5.5 (see Equation (5.5.1)) to obtain an orthonormal collection of m Bloch vectors $\{\psi_a\}_{a=1}^m$ for $\{P(\mathbf{k})\}_{\mathbf{k} \in \mathbb{R}^2}$ which are continuous and \mathbb{Z} -periodic in the variable k_2 . The continuous and periodic family of unitary matrices $\{\alpha_{2D}(k_2)\}_{k_2 \in \mathbb{R}}$, defined as in (5.5.2), measures the failure of $\{\psi_a\}_{a=1}^m$ to be periodic in k_1 .

Define

$$\tilde{\alpha}_{2D}(k_2) := \begin{pmatrix} \det \alpha_{2D}(k_2) & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{pmatrix}. \quad (5.6.1)$$

Clearly $\det \alpha_{2D}(k_2) = \det \tilde{\alpha}_{2D}(k_2)$, so that in particular α_{2D} and $\tilde{\alpha}_{2D}$ are homotopic. Proposition 5.6.3 applies and produces a family of unitary matrices $\{\beta_{2D}(k_1, k_2)\}_{(k_1, k_2) \in \mathbb{R}^2}$ which is periodic in k_2 and such that

$$\alpha_{2D}(k_2) = \beta_{2D}(k_1, k_2) \tilde{\alpha}_{2D}(k_2) \beta_{2D}(k_1 + 1, k_2)^{-1}$$

holds for all $(k_1, k_2) \in \mathbb{R}^2$.

With $\{\psi_a\}_{a=1}^m$ as in (5.5.1) and $\{\beta_{2D}(\mathbf{k})\}_{\mathbf{k} \in \mathbb{R}^2}$ as above, define

$$\xi_a(\mathbf{k}) := \sum_{b=1}^m \psi_b(\mathbf{k}) \beta_{2D}(\mathbf{k})_{ba}, \quad a \in \{1, \dots, m\}, \mathbf{k} \in \mathbb{R}^2.$$

Then we see that for $a \in \{1, \dots, m\}$ and $(k_1, k_2) \in \mathbb{R}^2$

$$\begin{aligned}
\xi_a(k_1 + 1, k_2) &= \sum_{b=1}^m \psi_b(k_1 + 1, k_2) \beta_{2D}(k_1 + 1, k_2)_{ba} \\
&= \sum_{b,c=1}^m \psi_c(k_1, k_2) \alpha_{2D}(k_2)_{cb} \beta_{2D}(k_1 + 1, k_2)_{ba} \\
&= \sum_{c=1}^m \psi_c(k_1, k_2) [\alpha_{2D}(k_2) \beta_{2D}(k_1 + 1, k_2)]_{ca} \\
&= \sum_{c=1}^m \psi_c(k_1, k_2) [\beta_{2D}(k_1, k_2) \tilde{\alpha}_{2D}(k_2)]_{ca} \\
&= \sum_{b=1}^m \sum_{c=1}^m \psi_c(k_1, k_2) \beta_{2D}(k_1, k_2)_{cb} \tilde{\alpha}_{2D}(k_2)_{ba} = \sum_{b=1}^m \xi_b(k_1, k_2) \tilde{\alpha}_{2D}(k_2)_{ba}.
\end{aligned} \tag{5.6.2}$$

Since $\tilde{\alpha}_{2D}(k_2)$ is in the form (5.6.1), when we set $a \in \{2, \dots, m\}$ in the above equation this reads $\xi_a(k_1 + 1, k_2) = \xi_a(k_1, k_2)$, that is, $\{\xi_a\}_{a=2}^m$ is an orthonormal collection of $(m - 1)$ Bloch vectors which are continuous and \mathbb{Z}^2 -periodic. This concludes the proof of Theorem 5.3.2(i) in the 2-dimensional case.

We now move to the case $d = 3$. Let $\{P(\mathbf{k})\}_{\mathbf{k} \in \mathbb{R}^3}$ be a family of rank- m projections which is smooth and \mathbb{Z}^3 -periodic. In view of what we have just proved, the 2-dimensional restriction $\{P(0, k_2, k_3)\}_{(k_2, k_3) \in \mathbb{R}^2}$ admits a collection of m orthonormal Bloch vectors $\{\xi_a(0, \cdot, \cdot)\}_{a=1}^m$ satisfying

$$\begin{aligned}
\xi_1(0, k_2 + 1, k_3) &= \det \alpha_{2D}(k_3) \xi_1(0, k_2, k_3), \\
\xi_b(0, k_2 + 1, k_3) &= \xi_b(0, k_2, k_3) \text{ for all } b \in \{2, \dots, m\}, \\
\xi_a(0, k_2, k_3 + 1) &= \xi_a(0, k_2, k_3) \text{ for all } a \in \{1, \dots, m\}.
\end{aligned} \tag{5.6.3}$$

Parallel-transport these Bloch vectors along the k_1 -direction, and define $\{\psi_a\}_{a=1}^m$ as in (5.5.1) and $\{\alpha(k_2, k_3)\}_{(k_2, k_3) \in \mathbb{R}^2}$ as in (5.5.2). The latter matrices are still unitary, depend continuously on (k_2, k_3) , are periodic in k_3 , but

$$\alpha(k_2 + 1, k_3) = \tilde{\alpha}_{2D}(k_3) \alpha(k_2, k_3) \tilde{\alpha}_{2D}(k_3)^{-1},$$

as can be checked from (5.6.3). Thus, the family $\{\alpha(k_2, k_3)\}_{(k_2, k_3) \in \mathbb{R}^2}$ is $\tilde{\alpha}_{2D}$ -periodic, and consequently so is the family defined by

$$\tilde{\alpha}(k_2, k_3) := \begin{pmatrix} \det \alpha(k_2, k_3) & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{pmatrix}$$

(actually, since $\tilde{\alpha}$ and $\tilde{\alpha}_{2D}$ commute, in this case $\tilde{\alpha}_{2D}$ -periodicity reduces to mere periodicity). Since α and $\tilde{\alpha}$ share the same determinant, Proposition 5.6.3 again produces a continuous, $\tilde{\alpha}_{2D}$ -periodic family of unitary matrices $\{\beta(k_1, \mathbf{k})\}_{(k_1, \mathbf{k}) \in \mathbb{R}^3}$ such that for all $(k_1, \mathbf{k}) \in \mathbb{R}^3$

$$\alpha(\mathbf{k}) = \beta(k_1, \mathbf{k}) \tilde{\alpha}(\mathbf{k}) \beta(k_1 + 1, \mathbf{k})^{-1}.$$

Arguing as above (compare (5.6.2)), the collection of Bloch vectors defined by

$$\xi_a(k_1, \mathbf{k}) := \sum_{b=1}^m \psi_b(k_1, \mathbf{k}) \beta(k_1, \mathbf{k})_{ba}, \quad a \in \{1, \dots, m\}, \quad (k_1, \mathbf{k}) \in \mathbb{R}^3,$$

satisfies

$$\xi_a(k_1 + 1, \mathbf{k}) = \sum_{b=1}^m \xi_b(k_1, \mathbf{k}) \tilde{\alpha}(\mathbf{k})_{ba}, \quad a \in \{1, \dots, m\}.$$

Due to the form of $\tilde{\alpha}$, this implies again that $\{\xi_a\}_{a=2}^m$ are continuous, orthonormal, and \mathbb{Z}^3 -periodic Bloch vectors for $\{P(\mathbf{k})\}_{\mathbf{k} \in \mathbb{R}^3}$, thus concluding the proof. \square

5.7 Proof of Theorem 5.3.2(ii): moving Parseval frames of Bloch vectors

In this section, we finally prove Theorem 5.3.2(ii), and complete the proof of the first main result. The central step consists in proving the result for families of rank 1, which we will do first.

5.7.1 The rank-1 case

Proof of Theorem 5.3.2(ii) (rank-1 case). Let $d \leq 3$. We consider first a smooth and \mathbb{Z}^d -periodic family of projections $\{P_1(\mathbf{k})\}_{\mathbf{k} \in \mathbb{R}^d}$ of rank $m = 1$. We want to show that there exists two Bloch vectors $\{\xi_1, \xi_2\}$ which are continuous, \mathbb{Z}^d -periodic, and generate the 1-dimensional space $\text{Ran } P_1(\mathbf{k}) \subset \mathcal{H}$ at each $\mathbf{k} \in \mathbb{R}^d$.

To do so, fix a complex conjugation C on the Hilbert space \mathcal{H} (which is tantamount to the choice of an orthonormal basis). Define

$$Q(\mathbf{k}) := C P_1(-\mathbf{k}) C^{-1}. \quad (5.7.1)$$

Using the fact that C is an antiunitary operator such that $C^2 = \mathbf{1}$, one can check that $\{Q(\mathbf{k})\}_{\mathbf{k} \in \mathbb{R}^d}$ defines a smooth and \mathbb{Z}^d -periodic family of orthogonal projectors. Moreover, one also has that $c_1(Q)_{ij} = -c_1(P)_{ij}$ for all $1 \leq i < j \leq d$, as can be seen by integrating the identity

$$\text{Tr}_{\mathcal{H}}(Q(\mathbf{k}) [\partial_i Q(\mathbf{k}), \partial_j Q(\mathbf{k})]) = -\text{Tr}_{\mathcal{H}}(P_1(-\mathbf{k}) [\partial_i P_1(-\mathbf{k}), \partial_j P_1(-\mathbf{k})])$$

over \mathbb{T}_{ij}^2 (compare [89, 3]).

Set now $P(\mathbf{k}) := P_1(\mathbf{k}) \oplus Q(\mathbf{k})$ for $\mathbf{k} \in \mathbb{R}^d$. The rank-2 family of projections $\{P(\mathbf{k})\}_{\mathbf{k} \in \mathbb{R}^d}$ on $\mathcal{H} \oplus \mathcal{H}$ satisfies then

$$c_1(P)_{ij} = c_1(P_1)_{ij} + c_1(Q)_{ij} = 0 \quad \text{for all } 1 \leq i < j \leq d.$$

Hence, in view of the results of Section 5.5, it admits a Bloch basis $\{\psi_1, \psi_2\}$. Let $\pi_j: \mathcal{H} \oplus \mathcal{H} \rightarrow \mathcal{H}$ be the projection on the j -th factor, $j \in \{1, 2\}$. Set finally

$$\xi_a(\mathbf{k}) := \pi_1((P_1(\mathbf{k}) \oplus 0) \psi_a(\mathbf{k})), \quad a \in \{1, 2\}, \quad \mathbf{k} \in \mathbb{R}^d.$$

Let us show that $\{\xi_a(\mathbf{k})\}_{a=1}^2$ gives a (continuous and \mathbb{Z}^d -periodic) Parseval frame in $\text{Ran } P_1(\mathbf{k})$. Indeed, let $\psi \in \text{Ran } P_1(\mathbf{k})$: then automatically $\psi \oplus 0 \in \text{Ran } P(\mathbf{k})$. Since $\{\psi_a(\mathbf{k})\}_{a=1}^2$ is an orthonormal basis for $\text{Ran } P(\mathbf{k})$, we obtain that

$$\psi \oplus 0 = \sum_{a=1}^2 \langle \psi_a(\mathbf{k}), \psi \oplus 0 \rangle_{\mathcal{H} \oplus \mathcal{H}} \psi_a(\mathbf{k}) = \sum_{a=1}^2 \langle \xi_a(\mathbf{k}), \psi \rangle_{\mathcal{H}} \psi_a(\mathbf{k}).$$

Finally, we apply $\pi_1 \circ (P_1(\mathbf{k}) \oplus 0)$ on both sides and obtain

$$\psi = \sum_{a=1}^2 \langle \xi_a(\mathbf{k}), \psi \rangle_{\mathcal{H}} \xi_a(\mathbf{k})$$

which is the defining condition (5.3.1) for $\{\xi_a(\mathbf{k})\}_{a=1}^2$ to be a Parseval frame in $\text{Ran } P_1(\mathbf{k})$. \square

5.7.2 The higher rank case: $m > 1$

Proof of Theorem 5.3.2(ii) (rank- m case, $m > 1$). Let $d \leq 3$, and consider a smooth and \mathbb{Z}^d -periodic family of rank- m projections $\{P(\mathbf{k})\}_{\mathbf{k} \in \mathbb{R}^d}$. In view of Theorem 5.3.2(i), which we already proved, it admits $m - 1$ orthonormal Bloch vectors $\{\xi_a\}_{a=1}^{m-1}$: they are \mathbb{Z}^d -periodic, and without loss of generality (see Appendix A.2.1) we assume them to be smooth. Denote by

$$P_{m-1}(\mathbf{k}) := \sum_{a=1}^{m-1} |\xi_a(\mathbf{k})\rangle \langle \xi_a(\mathbf{k})|, \quad \mathbf{k} \in \mathbb{R}^d,$$

the rank- $(m - 1)$ projection onto the space spanned by $\{\xi_a(\mathbf{k})\}_{a=1}^{m-1}$. Since the latter are smooth and periodic Bloch vectors for $\{P(\mathbf{k})\}_{\mathbf{k} \in \mathbb{R}^d}$, the family $\{P_{m-1}(\mathbf{k})\}_{\mathbf{k} \in \mathbb{R}^d}$ is smooth, \mathbb{Z}^d -periodic, and satisfies $P_{m-1}(\mathbf{k}) P(\mathbf{k}) = P(\mathbf{k}) P_{m-1}(\mathbf{k}) = P_{m-1}(\mathbf{k})$.

Denote by $P_1(\mathbf{k})$ the orthogonal projection onto the orthogonal complement of $\text{Ran } P_{m-1}(\mathbf{k})$ inside $\text{Ran } P(\mathbf{k})$. Then $\{P_1(\mathbf{k})\}_{\mathbf{k} \in \mathbb{R}^d}$ is a smooth and \mathbb{Z}^d -periodic family of rank-1 projections, and furthermore $P_1(\mathbf{k}) P(\mathbf{k}) = P(\mathbf{k}) P_1(\mathbf{k}) = P_1(\mathbf{k})$. In view of the results of the previous Subsections, we can construct two continuous and \mathbb{Z}^d -periodic Bloch vectors $\{\xi_m, \xi_{m+1}\}$ which generate $\text{Ran } P_1(\mathbf{k})$ at all $\mathbf{k} \in \mathbb{R}^d$. Since $P_1(\mathbf{k})$ is a sub-projection of $P(\mathbf{k})$, it then follows that

$$P(\mathbf{k}) \xi_a(\mathbf{k}) = P(\mathbf{k}) P_1(\mathbf{k}) \xi_a(\mathbf{k}) = P_1(\mathbf{k}) \xi_a(\mathbf{k}) = \xi_a(\mathbf{k}) \quad \text{for all } a \in \{m, m+1\}.$$

Besides, by construction $\{\xi_m(\mathbf{k}), \xi_{m+1}(\mathbf{k})\}$ generate the orthogonal complement in $\text{Ran } P(\mathbf{k})$ to the span of $\{\xi_a(\mathbf{k})\}_{a=1}^{m-1}$, and hence the full collection of $m + 1$ Bloch vectors $\{\xi_a\}_{a=1}^{m+1}$ give an $(m + 1)$ -frame for $\{P(\mathbf{k})\}_{\mathbf{k} \in \mathbb{R}^d}$ consisting of continuous and \mathbb{Z}^d -periodic vectors, as desired. \square

5.8 Proof of Theorem 5.4.1: from Hofstadter-like Hamiltonians to Fermi-like magnetic projections

In this section we leave the periodic setting and start the proof of Theorem 5.4.1, which applies to a 2-dimensional discrete magnetic Hamiltonian H_b , as described

in Section 5.2 (from which we borrow much of the notation). We show that, in order to exhibit an exponentially localized Wannier Parseval frame for the the Fermi projection of the original Hamiltonian, it is sufficient to solve the same problem for a suitable family of *Fermi-like magnetic projections*, in the sense of Definition 5.8.2 and Lemma 5.8.4 below.

5.8.1 Fermi-like magnetic projections

In the following, we drop the dependence on q for notational convenience, effectively setting $q = 1$ in the magnetic phase $e^{iq\phi(\cdot)}$.

We assume that H_{b_0} , and hence $\tilde{\mathcal{H}}_0 \equiv U_{b_0} H_{b_0} U_{b_0}^*$, has an isolated spectral island. Then we know that there exists ϵ^* such that for every $\epsilon \leq \epsilon^*$ also $\tilde{\mathcal{H}}_\epsilon$ has an isolated spectral island [29]. This allows us to define the family of spectral projections onto this spectral island of $\tilde{\mathcal{H}}_\epsilon$, that we denote by $\{\tilde{\mathcal{P}}_\epsilon\}_{0 \leq \epsilon \leq \epsilon^*}$. In the following, we will show that there exists an $\epsilon_0 < \epsilon^*$ such that $\tilde{\mathcal{P}}_\epsilon$ admits a Parseval frames in the sense of Theorem 5.4.1, for every $\epsilon < \epsilon_0$. Notice that this implies also the existence of a Parseval frame for the Fermi projection $\Pi_{b=b_0+\epsilon}$ of the original Hamiltonian $H_{b=b_0+\epsilon}$ consisting of exponentially localized generalized Wannier functions, since the two projections $\Pi_{b=b_0+\epsilon}$ and $\tilde{\mathcal{P}}_\epsilon$ are unitarily conjugated by the explicit unitary multiplication operator $U_{b=b_0+\epsilon}$ in (5.2.4), see Corollary 5.4.3.

From (5.2.3) we see that the ϵ -dependence of (the matrix elements of) the Hamiltonian $\tilde{\mathcal{H}}_\epsilon$ is both in the phase factor and in $h_{\mathbf{k},\epsilon}$. Nevertheless, it is easier to remove the latter dependence; we will see that this does not spoil the validity of Theorem 5.4.1. We thus consider the operator \mathcal{H}_ϵ acting on $\ell^2(\mathbb{Z}^2) \otimes \mathbb{C}^Q$ defined by the matrix elements

$$\begin{aligned} \mathcal{H}_\epsilon(\gamma, \underline{x}; \gamma', \underline{x}') &:= e^{i\epsilon\phi(\gamma, \gamma')} \mathcal{T}_0(\gamma - \gamma'; \underline{x}, \underline{x}'), \\ \text{where } \mathcal{T}_0(\gamma; \underline{x}, \underline{x}') &:= \int_{\Omega} d\mathbf{k} e^{i2\pi\mathbf{k}\cdot\gamma} h_{\mathbf{k},0}(\underline{x}, \underline{x}') \end{aligned} \quad (5.8.1)$$

for $\gamma, \gamma' \in \mathbb{Z}^2$ and $\underline{x}, \underline{x}' \in \{1, \dots, Q\}$. Notice that, in view of Remark 5.2.2, \mathcal{H}_ϵ still commutes with the magnetic translations $\tau_{\epsilon, \eta}$, $\eta \in \mathbb{Z}^2$, defined in (5.2.10).

The following lemma ensures that if $\tilde{\mathcal{H}}_\epsilon$ is gapped, also \mathcal{H}_ϵ is gapped.

Lemma 5.8.1. *There exists $\tilde{\epsilon}_0$ such that, for every $0 \leq \epsilon \leq \tilde{\epsilon}_0$, the spectral island $\sigma_{b_0+\epsilon}$ of \mathcal{H}_ϵ is ϵ -close in the Hausdorff distance to a spectral island $\tilde{\sigma}_{b_0+\epsilon}$ of $\tilde{\mathcal{H}}_\epsilon$.*

Proof. From (5.2.5) we see that

$$\left| \mathcal{H}_\epsilon(\gamma, \underline{x}; \gamma', \underline{x}') - \tilde{\mathcal{H}}_\epsilon(\gamma, \underline{x}; \gamma', \underline{x}') \right| \leq C \epsilon (\|\gamma - \gamma'\| + 1) |\mathcal{T}(\gamma - \gamma'; \underline{x}, \underline{x}')|,$$

which implies the estimate

$$\left| \mathcal{H}_\epsilon(\gamma, \underline{x}; \gamma', \underline{x}') - \tilde{\mathcal{H}}_\epsilon(\gamma, \underline{x}; \gamma', \underline{x}') \right| \leq C \epsilon e^{-\beta\|\gamma - \gamma'\|} \quad (5.8.2)$$

for some positive constants $C, \beta > 0$ uniformly in $\underline{x}, \underline{x}' \in \{1, \dots, Q\}$. From the above we conclude via a Schur–Holmgren estimate that $\|\mathcal{H}_\epsilon - \tilde{\mathcal{H}}_\epsilon\| \leq C' \epsilon$ for some constant $C' > 0$. An elementary argument based on Neumann series shows that if $\text{dist}(z, \sigma(\mathcal{H}_\epsilon)) > C' \epsilon$ then z must also be in the resolvent set of $\tilde{\mathcal{H}}_\epsilon$. The argument is symmetric in the two operators, hence the spectra are at Hausdorff distance ϵ . \square

In view of the above lemma, the family of projections $\{\mathcal{P}_\epsilon\}_{\epsilon \in [0, \tilde{\epsilon}_0]}$ onto the spectral island $\sigma_{b_0+\epsilon}$ of \mathcal{H}_ϵ is well defined, for example by the Riesz formula

$$\mathcal{P}_\epsilon = \frac{i}{2\pi} \oint_{\mathcal{C}} dz (\mathcal{H}_\epsilon - z)^{-1}, \quad (5.8.3)$$

where \mathcal{C} is a positively-oriented contour in the complex energy plane which encloses only the spectral island $\sigma_{b_0+\epsilon}$. This family of projections satisfies a number of properties (see Proposition 5.8.3 below), which for later convenience we collect in the following Definition.

Definition 5.8.2 (Fermi-like magnetic projections). A family of projections $\{\Pi^{(\epsilon)}\}_{\epsilon \in [0, \epsilon_0]}$ acting on $\ell^2(\mathbb{Z}^2) \otimes \mathbb{C}^Q$ is called a family of *Fermi-like magnetic projections* if the following properties are satisfied:

- (i) *perturbation of a periodic projection:* the projection $\Pi_0 \equiv \Pi^{(0)}$ is such that there exists a family of rank- m orthogonal projection $P_0(\mathbf{k})$ acting on \mathbb{C}^Q which is smooth and \mathbb{Z}^2 -periodic as a function of \mathbf{k} , and such that

$$\Pi_0(\gamma, \underline{x}; \gamma', \underline{x}') = \int_{\Omega} d\mathbf{k} e^{i2\pi\mathbf{k} \cdot (\gamma - \gamma')} P_0(\mathbf{k})(\underline{x}, \underline{x}') \quad (5.8.4)$$

for all $\gamma, \gamma' \in \mathbb{Z}^2$, $\underline{x}, \underline{x}' \in \{1, \dots, Q\}$; moreover for some positive constants C and α

$$\left| \Pi^{(\epsilon)}(\gamma, \underline{x}; \gamma', \underline{x}') - e^{i\epsilon\phi(\gamma, \gamma')} \Pi_0(\gamma, \underline{x}; \gamma', \underline{x}') \right| \leq C \epsilon e^{-\alpha\|\gamma - \gamma'\|} \quad (5.8.5)$$

for all $\gamma, \gamma' \in \mathbb{Z}^2$ and $\underline{x}, \underline{x}' \in \{1, \dots, Q\}$;

- (ii) *exponential localization of the matrix elements:* for some positive constants C and λ we have

$$\left| \Pi^{(\epsilon)}(\gamma, \underline{x}; \gamma', \underline{x}') \right| \leq C e^{-\lambda\|\gamma - \gamma'\|} \quad (5.8.6)$$

for all $\gamma, \gamma' \in \mathbb{Z}^2$, $\underline{x}, \underline{x}' \in \{1, \dots, Q\}$ and $\epsilon \in [0, \epsilon_0]$;

- (iii) *intertwining with the magnetic translations:* for all $\eta \in \mathbb{Z}^2$

$$e^{i\epsilon\phi(\gamma, \eta)} \Pi^{(\epsilon)}(\gamma - \eta, \underline{x}; \gamma' - \eta, \underline{x}') e^{-i\epsilon\phi(\gamma', \eta)} = \Pi^{(\epsilon)}(\gamma, \underline{x}; \gamma', \underline{x}') \quad (5.8.7)$$

for all $\gamma, \gamma' \in \mathbb{Z}^2$ and $\underline{x}, \underline{x}' \in \{1, \dots, Q\}$.

Notice that the above relation (5.8.7) is clearly equivalent to

$$\tau_{\epsilon, \eta} \Pi^{(\epsilon)} \tau_{\epsilon, \eta}^* = \Pi^{(\epsilon)}, \quad \forall \eta \in \mathbb{Z}^2 \quad (5.8.8)$$

by a computation analogous to (5.2.11).

Proposition 5.8.3. *The family of projections $\{\mathcal{P}_\epsilon\}_{\epsilon \in [0, \tilde{\epsilon}_0]}$ is a family of magnetic Fermi-like projections in the sense of Definition 5.8.2.*

Proof. Since \mathcal{H}_ϵ commutes with the magnetic translations, every \mathcal{P}_ϵ satisfies (5.8.7) by construction. Moreover, they also satisfy (5.8.6). This is a direct application of the Combes–Thomas estimates on the resolvent of \mathcal{H}_ϵ , because the gap in the spectrum of the Hamiltonian persists for every ϵ . For completeness we report the proof of the Combes–Thomas estimates in Appendix A.2.5, see Proposition A.2.7.

By hypothesis, $\mathcal{H}_0 = \tilde{\mathcal{H}}_0$ has a (possibly) non-trivial spectral island σ_{b_0} which must come from the ranges of $m < Q$ bands of $h_{\mathbf{k},0}$. In other words, $h_{\mathbf{k},0}$ has $m < Q$ eigenvalues whose ranges remain separated from the other $Q - m$, and these ranges together build up the spectral island σ_{b_0} . Denote by $P_0(\mathbf{k})$ the spectral projection of $h_{\mathbf{k},0}$ corresponding to these m eigenvalues. From the properties of $h_{\mathbf{k},0}$ we can deduce that $P_0(\mathbf{k})$ is smooth and periodic in \mathbf{k} , and the spectral projection of \mathcal{H}_0 onto σ_{b_0} is simply given by

$$\mathcal{P}_0(\gamma, \underline{x}; \gamma', \underline{x}') = \int_{\Omega} d\mathbf{k} e^{i2\pi\mathbf{k}\cdot(\gamma-\gamma')} P_0(\mathbf{k})(\underline{x}, \underline{x}'), \quad \gamma, \gamma' \in \mathbb{Z}^2, \underline{x}, \underline{x}' \in \{1, \dots, Q\}.$$

Hence also the property (5.8.4) is proved.

Now it remains to prove (5.8.5). This result is essentially known, see [29] and [21]; for completeness, we present a proof adapted to our setting in Proposition A.2.8. \square

Coming back to the problem of constructing a Parseval frame spanning the range of the Fermi projection $\tilde{\mathcal{P}}_\epsilon$ of $\tilde{\mathcal{H}}_\epsilon$, we show that it is in fact sufficient to construct it for the Fermi-like magnetic projections \mathcal{P}_ϵ .

Lemma 5.8.4. *There exists $\epsilon_0 \leq \tilde{\epsilon}_0$ such that, for every $0 \leq \epsilon \leq \epsilon_0$, the Fermi-like magnetic projection \mathcal{P}_ϵ admits a magnetic Parseval frame in the sense of Theorem 5.4.1 if and only if the Fermi projection $\tilde{\mathcal{P}}_\epsilon$ admits it.*

Proof. The two families $\{\mathcal{P}_\epsilon\}_{\epsilon \in [0, \tilde{\epsilon}_0]}$ and $\{\tilde{\mathcal{P}}_\epsilon\}_{\epsilon \in [0, \tilde{\epsilon}_0]}$ are projections onto isolated spectral island of Hamiltonians with exponentially localized matrix elements (see Proposition A.2.7), and hence have themselves exponentially localized matrix elements in view of the Riesz formula (5.8.3) (compare (5.8.6)). Using the resolvent identity and (5.8.2), it follows that

$$\left| \mathcal{P}_\epsilon(\gamma, \underline{x}; \gamma', \underline{x}') - \tilde{\mathcal{P}}_\epsilon(\gamma, \underline{x}; \gamma', \underline{x}') \right| \leq C \epsilon e^{-\beta \|\gamma - \gamma'\|}. \quad (5.8.9)$$

Because of this, there exists an $\epsilon_0 > 0$ such that $\|\mathcal{P}_\epsilon - \tilde{\mathcal{P}}_\epsilon\| \leq 1/2$ for all $\epsilon \leq \epsilon_0$. Then via the associated Kato–Nagy unitary K_ϵ [64] we have $\tilde{\mathcal{P}}_\epsilon = K_\epsilon \mathcal{P}_\epsilon K_\epsilon^{-1}$. The formula

$$\begin{aligned} K_\epsilon &= \left[\mathbf{1} - (\tilde{\mathcal{P}}_\epsilon - \mathcal{P}_\epsilon)^2 \right]^{-1/2} \left(\tilde{\mathcal{P}}_\epsilon \mathcal{P}_\epsilon + (\mathbf{1} - \tilde{\mathcal{P}}_\epsilon)(\mathbf{1} - \mathcal{P}_\epsilon) \right) \\ &= \left[\mathbf{1} + \sum_{k=1}^{\infty} \frac{(2k-1)!!}{k!2^k} (\tilde{\mathcal{P}}_\epsilon - \mathcal{P}_\epsilon)^{2k} \right] \left(\tilde{\mathcal{P}}_\epsilon \mathcal{P}_\epsilon + (\mathbf{1} - \tilde{\mathcal{P}}_\epsilon)(\mathbf{1} - \mathcal{P}_\epsilon) \right) \end{aligned} \quad (5.8.10)$$

for the Kato–Nagy unitary clearly shows that also K_ϵ commutes with the magnetic translations. Thus we see that if $\{w_a^{(\epsilon)}\}_{1 \leq a \leq M}$ is such that (5.4.1) holds then the vectors $\{K_\epsilon^* w_a^{(\epsilon)}\}_{1 \leq a \leq M}$ will span (together with all their magnetic translates) the range of \mathcal{P}_ϵ , and viceversa. In order to see that the vectors $K_\epsilon^* w_a^{(\epsilon)} = w_a^{(\epsilon)} +$

$(K_\epsilon^* - \mathbf{1})w_a^{(\epsilon)}$ are also exponentially localized, it suffices to show that $K_\epsilon - \mathbf{1}$ has exponentially localized matrix elements in the sense of (5.8.6), which we will do below in Lemma 5.8.5. This will conclude the proof. \square

Lemma 5.8.5. *For K_ϵ in (5.8.10), there exist constants $C, \lambda > 0$ such that for all $\gamma, \gamma' \in \mathbb{Z}^2$ and $\underline{x}, \underline{x}' \in \{1, \dots, Q\}$ and if ϵ is small enough*

$$|K_\epsilon(\gamma, \underline{x}; \gamma', \underline{x}') - \delta_{\gamma, \gamma'} \delta_{\underline{x}, \underline{x}'}| \leq C e^{-\lambda \|\gamma - \gamma'\|}.$$

Proof. Using $\tilde{\mathcal{P}}_\epsilon = \tilde{\mathcal{P}}_\epsilon^2$ and $\mathcal{P}_\epsilon = \mathcal{P}_\epsilon^2$, let us first rewrite (5.8.10) as

$$\begin{aligned} K_\epsilon - \mathbf{1} &= 2\tilde{\mathcal{P}}_\epsilon \mathcal{P}_\epsilon - \tilde{\mathcal{P}}_\epsilon - \mathcal{P}_\epsilon \\ &+ \left[\sum_{k=1}^{\infty} \frac{(2k-1)!!}{k!2^k} (\tilde{\mathcal{P}}_\epsilon - \mathcal{P}_\epsilon)^{2k} \right] (\tilde{\mathcal{P}}_\epsilon \mathcal{P}_\epsilon + (\mathbf{1} - \tilde{\mathcal{P}}_\epsilon)(\mathbf{1} - \mathcal{P}_\epsilon)) \\ &= \tilde{\mathcal{P}}_\epsilon (\mathcal{P}_\epsilon - \tilde{\mathcal{P}}_\epsilon) + (\mathcal{P}_\epsilon - \tilde{\mathcal{P}}_\epsilon) \mathcal{P}_\epsilon \\ &+ \left[\sum_{k=1}^{\infty} \frac{(2k-1)!!}{k!2^k} (\tilde{\mathcal{P}}_\epsilon - \mathcal{P}_\epsilon)^{2k} \right] (\tilde{\mathcal{P}}_\epsilon \mathcal{P}_\epsilon + (\mathbf{1} - \tilde{\mathcal{P}}_\epsilon)(\mathbf{1} - \mathcal{P}_\epsilon)). \end{aligned} \quad (5.8.11)$$

The right-hand side of the above is a sum of operators which are all expressed in terms of $D_\epsilon := \tilde{\mathcal{P}}_\epsilon - \mathcal{P}_\epsilon$ times the bounded operators \mathcal{P}_ϵ , $\tilde{\mathcal{P}}_\epsilon$ and $\tilde{\mathcal{P}}_\epsilon \mathcal{P}_\epsilon + (\mathbf{1} - \tilde{\mathcal{P}}_\epsilon)(\mathbf{1} - \mathcal{P}_\epsilon)$. Notice that, in view of (5.8.9), we have

$$|D_\epsilon(\gamma, \underline{x}; \gamma', \underline{x}')| \leq C \epsilon e^{-\beta \|\gamma - \gamma'\|}, \quad \gamma, \gamma' \in \mathbb{Z}^2, \underline{x}, \underline{x}' \in \{1, \dots, Q\}. \quad (5.8.12)$$

Thus, to show that the matrix elements of $K_\epsilon - \mathbf{1}$ satisfy the estimate in the statement, it suffices to show that the series in square brackets appearing in (5.8.11) defines an operator O_ϵ with exponentially localized matrix elements.

Consider the matrix elements of D_ϵ^n with $n \in \mathbb{N}$ and $n \geq 2$:

$$D_\epsilon^n(\gamma, \underline{x}; \gamma', \underline{x}') = \sum_{\gamma_1 \in \mathbb{Z}^2} \sum_{\underline{x}_1=1}^Q \cdots \sum_{\gamma_{n-1} \in \mathbb{Z}^2} \sum_{\underline{x}_{n-1}=1}^Q D_\epsilon(\gamma, \underline{x}; \gamma_1, \underline{x}_1) \cdots D_\epsilon(\gamma_{n-1}, \underline{x}_{n-1}; \gamma', \underline{x}').$$

In view of (5.8.12) we have that, for $0 < \beta' < \beta$,

$$\begin{aligned} &e^{\beta' \|\gamma - \gamma'\|} |D_\epsilon^n(\gamma, \underline{x}; \gamma', \underline{x}')| \\ &\leq C \epsilon Q^{n-1} \left(\sup_{\gamma'' \in \mathbb{Z}^2} \sup_{\underline{x}'', \underline{y} \in \{1, \dots, Q\}} \sum_{\eta \in \mathbb{Z}^2} |D_\epsilon(\gamma'', \underline{x}''; \eta, \underline{y})| e^{\beta' \|\gamma'' - \eta\|} \right)^{n-1} \\ &\leq \epsilon^n (C')^n \end{aligned}$$

for some $C' > 0$. With this estimate, it follows that

$$|O_\epsilon(\gamma, \underline{x}; \gamma', \underline{x}')| \leq [(1 - (\epsilon C'))^{-1/2} - 1] e^{-\beta' \|\gamma - \gamma'\|} \leq C'' \epsilon e^{-\beta' \|\gamma - \gamma'\|}$$

for some $C'' > 0$ uniform in $\gamma, \gamma' \in \mathbb{Z}^2$, $\underline{x}, \underline{x}' \in \{1, \dots, Q\}$, and ϵ sufficiently small. \square

5.9 Proof of Theorem 5.4.1: Parseval frames for Fermi-like magnetic projections

In view of the discussion in the previous section, we have reduced the statement of Theorem 5.4.1 to the following equivalent result, formulated in terms of Fermi-like magnetic projections.

Proposition 5.9.1. *Let $\{\Pi^{(\epsilon)}\}_{\epsilon \in [0, \epsilon_0]}$ be a family of Fermi-like magnetic projections as in Definition 5.8.2. Then there exists $\epsilon'_0 < \epsilon_0$ such that for all $0 \leq \epsilon \leq \epsilon'_0$ the following hold:*

- (i) *one can construct $m-1$ orthonormal exponentially localized vectors $\{w_s^{(\epsilon)}\}_{1 \leq s \leq m-1}$ and two other exponentially localized vectors $\{W_r^{(\epsilon)}\}_{1 \leq r \leq 2}$ such that*

$$\begin{aligned}\Pi_1^{(\epsilon)} &:= \sum_{\gamma \in \mathbb{Z}^2} \sum_{s=1}^{m-1} \left| \tau_{\epsilon, \gamma} w_s^{(\epsilon)} \right\rangle \left\langle \tau_{\epsilon, \gamma} w_s^{(\epsilon)} \right|, \\ \Pi_2^{(\epsilon)} &:= \sum_{\gamma \in \mathbb{Z}^2} \sum_{r=1}^2 \left| \tau_{\epsilon, \gamma} W_r^{(\epsilon)} \right\rangle \left\langle \tau_{\epsilon, \gamma} W_r^{(\epsilon)} \right|\end{aligned}$$

are two orthogonal projections commuting with all magnetic translations $\tau_{\epsilon, \gamma}$ defined in (5.2.10) and such that $\Pi^{(\epsilon)} = \Pi_1^{(\epsilon)} + \Pi_2^{(\epsilon)}$ and $\Pi_1^{(\epsilon)} \Pi_2^{(\epsilon)} = 0$;

- (ii) *if moreover $c_1(P_0) = 0 \in \mathbb{Z}$, where P_0 is as in (5.8.4), then one can construct m orthonormal and exponentially localized vectors $\{w_a^{(\epsilon)}\}_{1 \leq a \leq m}$ such that*

$$\Pi^{(\epsilon)} = \sum_{\gamma \in \mathbb{Z}^2} \sum_{a=1}^m \left| \tau_{\epsilon, \gamma} w_a^{(\epsilon)} \right\rangle \left\langle \tau_{\epsilon, \gamma} w_a^{(\epsilon)} \right|.$$

The rest of this section will be devoted to the proof of Proposition 5.9.1. Before diving into the mathematical details, we briefly sketch here the strategy of the case $c_1(P_0) \neq 0$, namely Proposition 5.9.1(i).

Step 1 By Definition 5.8.2 the projection $\Pi^{(0)}$ is a fibered operator in the Bloch–Floquet representation. Therefore, applying Theorem 5.3.2 we can construct an exponentially localized Wannier Parseval frame $\{\tau_{\epsilon=0, \gamma} w_a\}_{a \in \{1, \dots, m+1\}, \gamma \in \mathbb{Z}^2}$ for $\Pi^{(0)}$ (compare Theorem 5.3.4). Consider now the $m-1$ orthonormal exponentially localized Wannier vectors $\{w_s\}_{1 \leq s \leq m-1}$ together with all their magnetic translates via $\tau_{\epsilon, \gamma}$. Using gauge covariant magnetic perturbation theory by means of hypothesis (5.8.5), we can prove that the Gram matrix associated to the set $\{\Pi^{(\epsilon)} \tau_{\epsilon, \gamma} w_a\}_{a \in \{1, \dots, m-1\}, \gamma \in \mathbb{Z}^2}$ has matrix elements which decay exponentially away from the diagonal and is close to the identity. Hence we can construct $m-1$ orthogonal exponential localized vectors $\{w_s^{(\epsilon)}\}_{1 \leq s \leq m-1}$ in the range of Π^ϵ , such that $\Pi_1^{(\epsilon)} := \sum_{\gamma \in \mathbb{Z}^2} \sum_{s=1}^{m-1} \left| \tau_{\epsilon, \gamma} w_s^{(\epsilon)} \right\rangle \left\langle \tau_{\epsilon, \gamma} w_s^{(\epsilon)} \right|$.

Step 2 The second step makes use of the space-dimension-doubling procedure of Section 5.7 coupled with gauge covariant magnetic perturbation theory. We consider the operator $T^{(\epsilon)} = T_1^{(\epsilon)} \oplus T_2^{(\epsilon)}$ whose matrix elements are given by the matrix elements of the position-space representation of the projection $P_2(\mathbf{k}) \oplus (CP_2(\mathbf{k})C^{-1})$ times the ϵ -dependent Peierls magnetic phase $e^{i\epsilon\phi(\cdot)}$. $T^{(\epsilon)}$ is not a projection (for $\epsilon \neq 0$) but it is an almost projection, namely it is ϵ -close to an actual projection $\mathfrak{P}^{(\epsilon)} = \mathfrak{P}_1^{(\epsilon)} \oplus \mathfrak{P}_2^{(\epsilon)}$. Since the projection $T^{(\epsilon=0)}$ is trivial, we can repeat the procedure described in Step 1 and obtain a basis of exponentially localized Wannier-type functions for the projection $\mathfrak{P}^{(\epsilon)}$. Projecting onto one component of the doubled space and using a Kato–Nagy unitary K_ϵ , we obtain $\Pi_2^{(\epsilon)} = \sum_{\gamma \in \mathbb{Z}^2} \sum_{r=1}^2 |\tau_{\epsilon,\gamma} W_r^{(\epsilon)}\rangle \langle \tau_{\epsilon,\gamma} W_r^{(\epsilon)}|$, where $\Pi_2^{(\epsilon)} = K_\epsilon \mathfrak{P}_2^{(\epsilon)} K_\epsilon^{-1}$ and $\{W_r^{(\epsilon)}\}_{r \in \{1,2\}}$ are two exponentially localized vectors.

5.9.1 Parseval frame at $\epsilon = 0$

We first look at the projection $\Pi_0 \equiv \Pi^{(\epsilon=0)}$, which can be fibered through the projections $\{P_0(\mathbf{k})\}_{\mathbf{k} \in \mathbb{R}^2}$ as in (5.8.4). We know from Theorem 5.3.2 that we may find $m - 1$ orthonormal vectors $\{\xi_s(\mathbf{k})\}_{1 \leq s \leq m-1}$ in the range of $P_0(\mathbf{k})$ which are both \mathbb{Z}^2 -periodic and real-analytic in \mathbf{k} . Also, we may find two other vectors $\Xi_1(\mathbf{k})$ and $\Xi_2(\mathbf{k})$ in the range of $P_0(\mathbf{k})$ which are \mathbb{Z}^2 -periodic and real-analytic in \mathbf{k} , so that $\{\xi_1(\mathbf{k}), \dots, \xi_{m-1}(\mathbf{k}), \Xi_1(\mathbf{k}), \Xi_2(\mathbf{k})\}$ forms a Parseval frame for the range of $P_0(\mathbf{k})$. This means that we have the following orthogonal decomposition for $P_0(\mathbf{k})$:

$$\begin{aligned} P_0(\mathbf{k}) &= P_1(\mathbf{k}) + P_2(\mathbf{k}), \\ P_1(\mathbf{k}) &:= \sum_{s=1}^{m-1} |\xi_s(\mathbf{k})\rangle \langle \xi_s(\mathbf{k})|, \quad P_2(\mathbf{k}) := \sum_{r=1}^2 |\Xi_r(\mathbf{k})\rangle \langle \Xi_r(\mathbf{k})|. \end{aligned} \quad (5.9.1)$$

Note that $P_1(\mathbf{k})P_2(\mathbf{k}) = 0$ and $P_2(\mathbf{k})$ has rank 1. Going back from \mathbf{k} -space to position-space we define the operators Π_j acting in $\ell^2(\mathbb{Z}^2) \otimes \mathbb{C}^Q$ having the following matrix elements:

$$\begin{aligned} \Pi_j(\gamma, \underline{x}; \gamma', \underline{x}') &:= \int_{\Omega} d\mathbf{k} e^{i2\pi\mathbf{k} \cdot (\gamma - \gamma')} P_j(\mathbf{k})(\underline{x}, \underline{x}'), \\ j \in \{0, 1, 2\}, \gamma, \gamma' \in \mathbb{Z}^2, \underline{x}, \underline{x}' \in \{1, \dots, Q\}. \end{aligned}$$

Since $\Pi^{(\epsilon)}$ is a family of Fermi-like magnetic projections, from (5.8.6) we have

$$|\Pi_0(\gamma, \underline{x}; \gamma', \underline{x}')| \leq C \exp^{-\lambda \|\gamma - \gamma'\|}. \quad (5.9.2)$$

Define now the exponentially localized Wannier-type functions

$$w_s(\gamma, \underline{x}) := \int_{\Omega} d\mathbf{k} e^{i2\pi\mathbf{k} \cdot \gamma} \xi_s(\mathbf{k}, \underline{x}), \quad W_r(\gamma, \underline{x}) := \int_{\Omega} d\mathbf{k} e^{i2\pi\mathbf{k} \cdot \gamma} \Xi_r(\mathbf{k}, \underline{x}),$$

for $s \in \{1, \dots, m-1\}$ and $r \in \{1, 2\}$. Due to the analyticity of the Bloch-type vectors ξ_s and Ξ_r , we obtain that [42, 41, 71]

$$\begin{aligned} \max_{s \in \{1, \dots, m-1\}} \max_{\underline{x} \in \{1, \dots, Q\}} |e^{\beta \|\gamma\|} w_s(\gamma, \underline{x})| &\leq C, \\ \max_{r \in \{1, 2\}} \max_{\underline{x} \in \{1, \dots, Q\}} |e^{\beta \|\gamma\|} W_r(\gamma, \underline{x})| &\leq C; \end{aligned} \quad (5.9.3)$$

where β is less than the width of the strip of analyticity of the Bloch-type frame. Moreover we have the following identities:

$$\Pi_1 = \sum_{\gamma \in \mathbb{Z}^2} \sum_{s=1}^{m-1} |\tau_{0,\gamma} w_s\rangle \langle \tau_{0,\gamma} w_s|, \quad \Pi_2 = \sum_{\gamma \in \mathbb{Z}^2} \sum_{r=1}^2 |\tau_{0,\gamma} W_r\rangle \langle \tau_{0,\gamma} W_r|, \quad \Pi_0 = \Pi_1 + \Pi_2.$$

5.9.2 Construction of $\Pi_1^{(\epsilon)}$

The next lemma provides the construction of $\Pi_1^{(\epsilon)}$ as in the statement of Proposition 5.9.1.

Lemma 5.9.2 (Construction of $\Pi_1^{(\epsilon)}$). *Define the self-adjoint operator M_ϵ acting on the space $\ell^2(\mathbb{Z}^2) \otimes \mathbb{C}^{m-1}$ defined by the matrix elements*

$$M_\epsilon(\gamma, s; \gamma', s') := \left\langle \tau_{\epsilon,\gamma} w_s, \Pi^{(\epsilon)} \tau_{\epsilon,\gamma'} w_{s'} \right\rangle_{\ell^2(\mathbb{Z}^2) \otimes \mathbb{C}^Q}. \quad (5.9.4)$$

If ϵ_0 is small enough, then there exists some $C, \alpha > 0$ such that uniformly in $\epsilon \leq \epsilon_0$ we have

$$|\delta_{ss'} \delta_{\gamma\gamma'} - M_\epsilon(\gamma, s; \gamma', s')| \leq C \epsilon e^{-\alpha \|\gamma - \gamma'\|}. \quad (5.9.5)$$

The vectors

$$V_{\gamma'',s,\epsilon}(\gamma, \underline{x}) := \sum_{\gamma' \in \mathbb{Z}^2} \sum_{s'=1}^{m-1} [M_\epsilon^{-1/2}](\gamma', s'; \gamma'', s) [\Pi^{(\epsilon)} \tau_{\epsilon,\gamma'} w_{s'}](\gamma, \underline{x}) \quad (5.9.6)$$

are orthonormal. Moreover, there exist $m - 1$ exponentially localized vectors $w_s^{(\epsilon)}$, $s \in \{1, \dots, m - 1\}$, such that

$$V_{\gamma'',s,\epsilon} = \tau_{\epsilon,\gamma''} w_s^{(\epsilon)} \quad \text{for all } \gamma'' \in \mathbb{Z}^2, \epsilon \in [0, \epsilon_0]. \quad (5.9.7)$$

Finally

$$\Pi_1^{(\epsilon)} := \sum_{\gamma \in \mathbb{Z}^2} \sum_{s=1}^{m-1} |V_{\gamma,s,\epsilon}\rangle \langle V_{\gamma,s,\epsilon}| = \sum_{\gamma \in \mathbb{Z}^2} \sum_{s=1}^{m-1} \left| \tau_{\epsilon,\gamma} w_s^{(\epsilon)} \right\rangle \left\langle \tau_{\epsilon,\gamma} w_s^{(\epsilon)} \right|$$

is an orthogonal projection such that $\Pi^{(\epsilon)} \Pi_1^{(\epsilon)} = \Pi_1^{(\epsilon)}$.

Remark 5.9.3. When the Chern number of $\{P_0(\mathbf{k})\}_{\mathbf{k} \in \mathbb{R}^2}$ vanishes, then the construction of $\Pi_1^{(\epsilon)}$ provided by Lemma 5.9.2 above can be applied to the whole $\Pi^{(\epsilon)}$, thus proving also Proposition 5.9.1(ii).

Proof of Lemma 5.9.2. The proof follows the same ideas as in [30]. In the following the magnetic phase composition rule

$$\phi(\gamma, \gamma') + \phi(\gamma', \gamma'') = \phi(\gamma, \gamma'') + \phi(\gamma - \gamma', \gamma' - \gamma'') \quad (5.9.8)$$

will be used repeatedly. During the proof we will denote inessential constants by K .

Consider the operator $\widehat{\Pi}^{(\epsilon)}$ defined by the following matrix elements:

$$\begin{aligned}\widehat{\Pi}^{(\epsilon)}(\gamma, \underline{x}; \gamma', \underline{x}') &:= e^{i\epsilon\phi(\gamma, \gamma')} \Pi_0(\gamma, \underline{x}; \gamma', \underline{x}') \\ &= e^{i\epsilon\phi(\gamma, \gamma')} \Pi_1(\gamma, \underline{x}; \gamma', \underline{x}') + e^{i\epsilon\phi(\gamma, \gamma')} \Pi_2(\gamma, \underline{x}; \gamma', \underline{x}') \\ &=: \widehat{\Pi}_1^{(\epsilon)}(\gamma, \underline{x}; \gamma', \underline{x}') + \widehat{\Pi}_2^{(\epsilon)}(\gamma, \underline{x}; \gamma', \underline{x}'),\end{aligned}\quad (5.9.9)$$

and the operator $\widetilde{\Pi}^{(\epsilon)}$ defined by

$$\widetilde{\Pi}^{(\epsilon)} := \sum_{\gamma'' \in \mathbb{Z}^2} \sum_{s=1}^{m-1} |\tau_{\epsilon, \gamma''} w_s\rangle \langle \tau_{\epsilon, \gamma''} w_s| + \sum_{\gamma'' \in \mathbb{Z}^2} \sum_{r=1}^2 |\tau_{\epsilon, \gamma''} W_r\rangle \langle \tau_{\epsilon, \gamma''} W_r| =: \widetilde{\Pi}_1^{(\epsilon)} + \widetilde{\Pi}_2^{(\epsilon)}.\quad (5.9.10)$$

Then we have the following estimate:

$$\begin{aligned}|M_\epsilon(\gamma, s; \gamma', s') - \delta_{ss'} \delta_{\gamma\gamma'}| &\leq \left| \langle \tau_{\epsilon, \gamma} w_s, (\Pi^{(\epsilon)} - \widehat{\Pi}^{(\epsilon)}) \tau_{\epsilon, \gamma'} w_{s'} \rangle \right| \\ &\quad + \left| \langle \tau_{\epsilon, \gamma} w_s, (\widehat{\Pi}^{(\epsilon)} - \widetilde{\Pi}^{(\epsilon)}) \tau_{\epsilon, \gamma'} w_{s'} \rangle \right| \\ &\quad + \left| \langle \tau_{\epsilon, \gamma} w_s, \widetilde{\Pi}_2^{(\epsilon)} \tau_{\epsilon, \gamma'} w_{s'} \rangle \right| \\ &\quad + \left| \langle \tau_{\epsilon, \gamma} w_s, \widetilde{\Pi}_1^{(\epsilon)} \tau_{\epsilon, \gamma'} w_{s'} \rangle - \delta_{ss'} \delta_{\gamma\gamma'} \right|.\end{aligned}\quad (5.9.11)$$

The first term of the right-hand side is exponentially localized due to (5.8.5) and (5.9.3). In order to prove the exponential localization of the second term we prove an estimate analogue to (5.8.5) for the matrix elements of $\widehat{\Pi}^{(\epsilon)} - \widetilde{\Pi}^{(\epsilon)}$:

$$\begin{aligned}&\left| \widehat{\Pi}_1^{(\epsilon)}(\gamma, \underline{x}; \gamma', \underline{x}') - \widetilde{\Pi}_1^{(\epsilon)}(\gamma, \underline{x}; \gamma', \underline{x}') \right| \\ &\leq \sum_{\gamma'' \in \mathbb{Z}^2} \sum_{s'=1}^{m-1} \left| \left(1 - e^{i\epsilon\phi(\gamma - \gamma'', \gamma'' - \gamma')} \right) w_{s''}(\gamma - \gamma'', \underline{x}) \overline{w_{s''}(\gamma' - \gamma'', \underline{x}')} \right| \\ &\leq \frac{\epsilon}{2} \sum_{\gamma'' \in \mathbb{Z}^2} \sum_{s'=1}^{m-1} \|\gamma - \gamma''\| \|\gamma'' - \gamma'\| \left| w_{s''}(\gamma - \gamma'', \underline{x}) \overline{w_{s''}(\gamma' - \gamma'', \underline{x}')} \right| \\ &\leq K \epsilon e^{-\alpha' \|\gamma - \gamma'\|},\end{aligned}\quad (5.9.12)$$

where $\alpha' < \beta$, since we have used (5.9.3). The same argument works also for the matrix elements of $\widehat{\Pi}_2^{(\epsilon)} - \widetilde{\Pi}_2^{(\epsilon)}$; hence we can conclude that

$$\left| \left(\widehat{\Pi}^{(\epsilon)} - \widetilde{\Pi}^{(\epsilon)} \right) (\gamma, \underline{x}; \gamma', \underline{x}') \right| \leq K \epsilon e^{-\alpha' \|\gamma - \gamma'\|}.$$

Then the exponential localization also of the second term on the right-hand side of (5.9.11) follows.

Consider now the scalar product $\langle \tau_{\epsilon, \gamma} w_s, \tau_{\epsilon, \gamma'} W_r \rangle$. Since $\tau_{0, \gamma} w_s$ and $\tau_{0, \gamma'} W_r$ belong to orthogonal subspaces for every $\gamma, \gamma' \in \mathbb{Z}^2$, $s \in \{1, \dots, m-1\}$ and $r \in$

$\{1, 2\}$, we have that

$$\begin{aligned}
 & |\langle \tau_{\epsilon, \gamma} w_s, \tau_{\epsilon, \gamma'} W_r \rangle| \\
 &= |\langle \tau_{\epsilon, \gamma} w_s, \tau_{\epsilon, \gamma'} W_r \rangle - \langle \tau_{0, \gamma} w_s, \tau_{0, \gamma'} W_r \rangle| \\
 &\leq \sum_{\gamma'' \in \mathbb{Z}^2} \sum_{\underline{y}=1}^Q \left| \left(e^{i\epsilon \phi(\gamma - \gamma'', \gamma'' - \gamma')} - 1 \right) \left| \overline{(\tau_{0, \gamma} w_s)(\gamma'', \underline{y})} (\tau_{0, \gamma'} W_r)(\gamma'', \underline{y}) \right| \right| \\
 &\leq e^{-\alpha \|\gamma - \gamma'\| \frac{\epsilon}{2}} \\
 &\quad \cdot \left(\sum_{\gamma'' \in \mathbb{Z}^2} \sum_{\underline{y}=1}^Q e^{\alpha \|\gamma - \gamma''\| \|\gamma'' - \gamma'\|} e^{\alpha \|\gamma'' - \gamma'\|} \left| \overline{(\tau_{0, \gamma} w_s)(\gamma'', \underline{y})} (\tau_{0, \gamma'} W_r)(\gamma'', \underline{y}) \right| \right) \\
 &\leq K \epsilon e^{-\alpha' \|\gamma - \gamma'\|}.
 \end{aligned} \tag{5.9.13}$$

The same argument works if we substitute $\tau_{\epsilon, \gamma'} W_r$ with $\tau_{\epsilon, \gamma'} w_{s'}$ as long as $(\gamma', s') \neq (\gamma, s)$. Thus we can also prove the exponential localization for the third term on the right-hand side of (5.9.11):

$$\begin{aligned}
 \left| \left\langle \tau_{\epsilon, \gamma} w_s, \tilde{\Pi}_2 \tau_{\epsilon, \gamma'} w_{s'} \right\rangle \right| &\leq \sum_{\gamma'' \in \mathbb{Z}^2} \sum_{r=1}^2 |\langle \tau_{\epsilon, \gamma} w_s, \tau_{\epsilon, \gamma''} W_r \rangle| |\langle \tau_{\epsilon, \gamma''} W_r, \tau_{\epsilon, \gamma'} w_{s'} \rangle| \\
 &\leq K' \epsilon^2 e^{-\alpha' \|\gamma - \gamma'\|} \sum_{\gamma'' \in \mathbb{Z}^2} \sum_{r=1}^2 e^{-\beta \|\gamma - \gamma''\|} \leq K \epsilon^2 e^{-\alpha'' \|\gamma - \gamma'\|},
 \end{aligned}$$

and for the fourth term as well:

$$\begin{aligned}
 & |\langle \tau_{\epsilon, \gamma} w_s, \tilde{\Pi}_1 \tau_{\epsilon, \gamma'} w_{s'} \rangle - \delta_{ss'} \delta_{\gamma\gamma'}| \\
 &\leq \delta_{\gamma\gamma'} \delta_{ss'} \sum_{\substack{(\gamma'', s'') \in \mathbb{Z}^2 \times \{1, \dots, m-1\} \\ (\gamma'', s'') \neq (\gamma, s)}} |\langle \tau_{\epsilon, \gamma} w_s, \tau_{\epsilon, \gamma''} w_{s''} \rangle| |\langle \tau_{\epsilon, \gamma''} w_{s''}, \tau_{\epsilon, \gamma'} w_{s'} \rangle| \\
 &\quad + \sum_{(\gamma'', s'') \in \mathbb{Z}^2 \times \{1, \dots, m-1\}} |\langle \tau_{\epsilon, \gamma} w_s, \tau_{\epsilon, \gamma''} w_{s''} \rangle| |\langle \tau_{\epsilon, \gamma''} w_{s''}, \tau_{\epsilon, \gamma'} w_{s'} \rangle| \\
 &\leq K \epsilon^2 e^{-\alpha'' \|\gamma - \gamma'\|},
 \end{aligned}$$

with $\alpha'' < \alpha'$. Hence (5.9.5) is proved.

Define now $D_\epsilon := M_\epsilon - \mathbf{1}$. The estimate (5.9.5) shows that the norm of D_ϵ is controlled by ϵ , therefore $M_\epsilon^{-1/2} = (\mathbf{1} + D_\epsilon)^{-1/2}$ exists and can be expressed as a norm convergent power series around $\epsilon = 0$. Moreover, arguing as in the proof of Lemma 5.8.5, one can show that $M_\epsilon^{-1/2}$ has exponentially localized matrix elements, and that

$$|M_\epsilon^{-1/2}(\gamma, s; \gamma', s') - \delta_{ss'} \delta_{\gamma\gamma'}| \leq C \epsilon e^{-\rho \|\gamma - \gamma'\|} \tag{5.9.14}$$

for some positive $C, \rho > 0$.

The series defined in (5.9.6) is now an absolutely convergent series and it is straightforward to check that the vectors $V_{\gamma'', s, \epsilon}$ form an orthonormal set. It remains to prove the existence of $m - 1$ exponentially localized vectors $w_s^{(\epsilon)}$ such that (5.9.7) holds. By hypothesis $\Pi^{(\epsilon)}$ satisfies (5.8.8), which together with (5.2.12) implies that

$$M_\epsilon(\gamma, s; \gamma', s') = \langle \tau_{\epsilon, \gamma} w_s, \tau_{\epsilon, \gamma'} \Pi^{(\epsilon)} w_{s'} \rangle = \langle \tau_{\epsilon, \gamma'}^* \tau_{\epsilon, \gamma} w_s, \Pi^{(\epsilon)} w_{s'} \rangle$$

$$\begin{aligned}
&= \left\langle e^{i\epsilon\phi(\gamma',\gamma)} \tau_{\epsilon,\gamma-\gamma'} w_s, \Pi^{(\epsilon)} w_{s'} \right\rangle = e^{i\epsilon\phi(\gamma,\gamma')} \left\langle \tau_{\epsilon,\gamma-\gamma'} w_s, \Pi^{(\epsilon)} w_{s'} \right\rangle \\
&=: e^{i\epsilon\phi(\gamma,\gamma')} m_\epsilon(\gamma - \gamma'; s, s').
\end{aligned}$$

By using the power series expansion for the inverse square root, one can prove (see [30]) a similar form for the matrix elements of $M_\epsilon^{-1/2}$, namely

$$[M_\epsilon^{-1/2}](\gamma, s; \gamma', s') =: e^{i\epsilon\phi(\gamma,\gamma')} m_{\epsilon,-1/2}(\gamma - \gamma'; s, s').$$

It then follows, using again (5.2.12) and (5.8.8), that

$$\begin{aligned}
V_{\gamma'',s,\epsilon} &= \sum_{\gamma' \in \mathbb{Z}^2} \sum_{s'=1}^{m-1} e^{i\epsilon\phi(\gamma',\gamma'')} m_{\epsilon,-1/2}(\gamma' - \gamma''; s', s) [\tau_{\epsilon,\gamma'} \Pi^{(\epsilon)} w_{s'}] \\
&= \sum_{\gamma = \gamma' - \gamma'' \in \mathbb{Z}^2} \sum_{s'=1}^{m-1} e^{i\epsilon\phi(\gamma+\gamma'',\gamma'')} m_{\epsilon,-1/2}(\gamma; s', s) [\tau_{\epsilon,\gamma+\gamma''} \Pi^{(\epsilon)} w_{s'}] \\
&= \sum_{\gamma \in \mathbb{Z}^2} \sum_{s'=1}^{m-1} e^{i\epsilon\phi(\gamma,\gamma'')} m_{\epsilon,-1/2}(\gamma; s', s) [e^{i\epsilon\phi(\gamma'',\gamma)} \tau_{\epsilon,\gamma''} \tau_{\epsilon,\gamma} \Pi^{(\epsilon)} w_{s'}] \\
&= \tau_{\epsilon,\gamma''} w_s^{(\epsilon)},
\end{aligned}$$

with

$$\begin{aligned}
w_s^{(\epsilon)} &:= \sum_{\gamma \in \mathbb{Z}^2} \sum_{s'=1}^{m-1} m_{\epsilon,-1/2}(\gamma; s', s) [\tau_{\epsilon,\gamma} \Pi^{(\epsilon)} w_{s'}] \\
&= \sum_{\gamma \in \mathbb{Z}^2} \sum_{s'=1}^{m-1} [M_\epsilon^{-1/2}](\gamma, s'; 0, s) [\tau_{\epsilon,\gamma} \Pi^{(\epsilon)} w_{s'}].
\end{aligned} \tag{5.9.15}$$

Due to the exponential localization (5.9.3) of the w_s 's and of the matrix elements of $M_\epsilon^{-1/2}$ and $\Pi^{(\epsilon)}$, we easily get that there exist $\beta', C > 0$, independent of \underline{x} , such that

$$\sup_{\gamma \in \mathbb{Z}^2} e^{\beta' \|\gamma\|} |w_s^{(\epsilon)}(\gamma, \underline{x})| \leq C. \tag{5.9.16}$$

□

Remark 5.9.4. Notice that the functions $w_s^{(\epsilon)}$ defined in (5.9.15) satisfy

$$\begin{aligned}
&w_s^{(\epsilon)} - w_{s'} \\
&= w_s^{(\epsilon)} - [\Pi_0 w_{s'}] = w_s^{(\epsilon)} - [\widehat{\Pi}^{(\epsilon)} w_{s'}] + [(\widehat{\Pi}^{(\epsilon)} - \Pi_0) w_{s'}] \\
&= \sum_{\eta \in \mathbb{Z}^2} \sum_{s''=1}^{m-1} [M_\epsilon^{-1/2}](\eta, s''; 0, s) [(\Pi^{(\epsilon)} - \delta_{0\eta} \delta_{s's''} \widehat{\Pi}^{(\epsilon)}) \tau_{\epsilon,\eta}] w_{s''} + [(\widehat{\Pi}^{(\epsilon)} - \Pi_0) w_{s'}]
\end{aligned}$$

hence

$$\begin{aligned}
 w_s^{(\epsilon)}(\gamma, \underline{x}) - w_{s'}(\gamma, \underline{x}) &= \sum_{\gamma' \in \mathbb{Z}^2} \sum_{\underline{x}'=1}^Q [M_\epsilon^{-1/2}](0, s'; 0, s) [\Pi^{(\epsilon)}(\gamma, \underline{x}; \gamma', \underline{x}') - e^{i\epsilon\phi(\gamma, \gamma')} \Pi_0(\gamma, \underline{x}; \gamma', \underline{x}')] w_{s'}(\gamma', \underline{x}') \\
 &+ \sum_{\eta \neq 0} \sum_{s'' \neq s'} \left([M_\epsilon^{-1/2}](\eta, s''; 0, s) - \delta_{0\eta} \delta_{s's''} \right) \\
 &\quad \cdot \sum_{\gamma' \in \mathbb{Z}^2} \sum_{\underline{x}'=1}^Q \Pi^{(\epsilon)}(\gamma, \underline{x}; \gamma', \underline{x}') e^{i\epsilon\phi(\gamma', \eta)} w_{s''}(\gamma' - \eta, \underline{x}') \\
 &+ \sum_{\gamma' \in \mathbb{Z}^2} \sum_{\underline{x}'=1}^Q (e^{i\epsilon\phi(\gamma, \gamma')} - 1) \Pi_0(\gamma, \underline{x}; \gamma', \underline{x}') w_{s'}(\gamma', \underline{x}').
 \end{aligned}$$

Using (5.8.5) to estimate the first sum on the right-hand side of the above, (5.9.14) with (5.8.6) for the second sum, and the power series of the exponential and (5.8.6) at $\epsilon = 0$ for the third sum, together with the exponential decay (5.9.3) of the functions w_s , we are able to deduce that for all $s, s' \in \{1, \dots, m-1\}$

$$|w_s^{(\epsilon)}(\gamma, \underline{x}) - w_{s'}(\gamma, \underline{x})| \leq C \epsilon e^{-\sigma \|\gamma\|}$$

for some positive constants $C, \sigma > 0$ uniform in $\gamma \in \mathbb{Z}^2$, $\underline{x} \in \{1, \dots, Q\}$, and ϵ sufficiently small. Clearly the above implies in turn that

$$|[\tau_{\epsilon, \eta} w_s^{(\epsilon)}](\gamma, \underline{x}) - [\tau_{\epsilon, \eta} w_{s'}](\gamma, \underline{x})| \leq C \epsilon e^{-\sigma \|\gamma - \eta\|} \quad (5.9.17)$$

for any $\eta \in \mathbb{Z}^2$.

5.9.3 Construction of $\Pi_2^{(\epsilon)}$

We now show that the orthogonal projection defined as

$$\Pi_2^{(\epsilon)} := \Pi^{(\epsilon)} - \Pi_1^{(\epsilon)} \quad (5.9.18)$$

can be written as in Proposition 5.9.1(i). To construct a Parseval frame for it we will mix the space-dimension-doubling method used in the proof of Theorem 5.3.2(iii) (see Section 5.7) with magnetic perturbation theory.

The projection $P_2(\mathbf{k})$ in (5.9.1) has rank 1, and we introduce $\tilde{P}_2(\mathbf{k}) := CP_2(-\mathbf{k})C^{-1}$ as in (5.7.1). Denote by $P_3(\mathbf{k}) := \tilde{P}_2(\mathbf{k}) \oplus P_2(\mathbf{k})$ the rank-2 projection acting on $\mathbb{C}^Q \oplus \mathbb{C}^Q$. As it is argued in Section 5.7, its Chern number is zero. We now define the operator

$$T^{(\epsilon)}(\gamma, \underline{x}; \gamma', \underline{x}') := e^{i\epsilon\phi(\gamma, \gamma')} \int_{\Omega} e^{i2\pi\mathbf{k} \cdot (\gamma - \gamma')} P_3(\mathbf{k})(\underline{x}, \underline{x}') d\mathbf{k},$$

for every $\gamma, \gamma' \in \mathbb{Z}^2$ and $\underline{x}, \underline{x}' \in \{1, \dots, 2Q\}$, acting on $\ell^2(\mathbb{Z}^2) \otimes (\mathbb{C}^Q \oplus \mathbb{C}^Q)$. Note the fact that $T^{(\epsilon)} = T_1^{(\epsilon)} \oplus T_2^{(\epsilon)}$ where $T_j^{(\epsilon)}$ acts on $\ell^2(\mathbb{Z}^2) \otimes \mathbb{C}^Q$. We also have

$$\begin{aligned}
 T_2^{(\epsilon)}(\gamma, \underline{x}; \gamma', \underline{x}') &:= e^{i\epsilon\phi(\gamma, \gamma')} \int_{\Omega} e^{i2\pi\mathbf{k} \cdot (\gamma - \gamma')} P_2(\mathbf{k})(\underline{x}, \underline{x}') d\mathbf{k} \\
 &= e^{i\epsilon\phi(\gamma, \gamma')} \Pi_2(\gamma, \underline{x}; \gamma', \underline{x}') = \hat{\Pi}_2^{(\epsilon)}(\gamma, \underline{x}; \gamma', \underline{x}'),
 \end{aligned} \quad (5.9.19)$$

for $\gamma, \gamma' \in \mathbb{Z}^2$ and $\underline{x}, \underline{x}' \in \{1, \dots, Q\}$, compare (5.9.9).

The operators $T_j^{(\epsilon)}$ are almost orthogonal projections, in the sense that

$$\Delta_j^{(\epsilon)} := \left\{ \left(T_j^{(\epsilon)} \right)^2 - T_j^{(\epsilon)} \right\} = \mathcal{O}(\epsilon)$$

in the operator norm; more precisely we want to prove an estimate of the usual type for the matrix elements of $\Delta_j^{(\epsilon)}$, namely

$$\left| \Delta_j^{(\epsilon)}(\gamma, \underline{x}; \gamma', \underline{x}') \right| \leq C \epsilon e^{-\alpha \|\gamma - \gamma'\|}. \quad (5.9.20)$$

In order to show this, notice first that $T_j^{(0)}$ is a true projection and hence $\Delta_j^{(0)} = 0$. Then, using the magnetic phase composition rule (5.9.8) to compute the matrix elements of $(T_j^{(\epsilon)})^2$ and noticing that

$$\left| T_j^{(\epsilon)}(\gamma; \underline{x}, \underline{x}') \right| \leq C e^{-\delta \|\gamma\|},$$

we obtain

$$\left| \Delta_j^{(\epsilon)}(\gamma, \underline{x}; \gamma', \underline{x}') \right| = \left| \Delta_j^{(\epsilon)}(\gamma, \underline{x}; \gamma', \underline{x}') - \Delta_j^{(0)}(\gamma, \underline{x}; \gamma', \underline{x}') \right| \leq C \epsilon e^{-\alpha \|\gamma - \gamma'\|}$$

as wanted.

Now if ϵ is small enough, we may construct the following explicit orthogonal projections acting on $\ell^2(\mathbb{Z}^2) \otimes \mathbb{C}^Q$ (see [87] for more details):

$$\mathfrak{P}_j^{(\epsilon)} := T_j^{(\epsilon)} + \left(T_j^{(\epsilon)} - \frac{1}{2} \mathbf{1} \right) \left\{ (\mathbf{1} + 4\Delta_j^{(\epsilon)})^{-1/2} - \mathbf{1} \right\}.$$

Simply using the above formula in each term of the direct sum in the expression for $T^{(\epsilon)}$ we obtain that

$$\mathfrak{P}^{(\epsilon)} = \mathfrak{P}_1^{(\epsilon)} \oplus \mathfrak{P}_2^{(\epsilon)}$$

is an orthogonal projection acting on the “doubled” space and, using (5.9.20) and arguing as in the proof of Lemma 5.8.5, that

$$\left| \mathfrak{P}^{(\epsilon)}(\gamma, \underline{x}; \gamma', \underline{x}') - T^{(\epsilon)}(\gamma, \underline{x}; \gamma', \underline{x}') \right| \leq C \epsilon e^{-\alpha \|\gamma - \gamma'\|}. \quad (5.9.21)$$

Because the non-magnetic projection $P_3(\mathbf{k})$ which builds up $T^{(\epsilon=0)}$ is trivial, mimicking the proof of Lemma 5.9.2 we infer that we can construct two exponentially localized Wannier-type vectors $F_r^{(\epsilon)} \in \ell^2(\mathbb{Z}^2) \otimes (\mathbb{C}^Q \oplus \mathbb{C}^Q)$ such that:

$$\mathfrak{P}^{(\epsilon)} = \sum_{\gamma \in \mathbb{Z}^2} \sum_{r=1}^2 \left| (\tau_{\epsilon, \gamma} \oplus \tau_{\epsilon, \gamma}) F_r^{(\epsilon)} \right\rangle \left\langle (\tau_{\epsilon, \gamma} \oplus \tau_{\epsilon, \gamma}) F_r^{(\epsilon)} \right|,$$

where $\tau_{\epsilon, \gamma} \oplus \tau_{\epsilon, \gamma}$ is the obvious extension of the magnetic translation to the doubled space. Restricting ourselves to vectors of the type $0 \oplus \psi$ where ψ is in the range of $\mathfrak{P}_2^{(\epsilon)}$, and denoting by $\pi_2: \ell^2(\mathbb{Z}^2) \otimes (\mathbb{C}^Q \oplus \mathbb{C}^Q) \rightarrow \ell^2(\mathbb{Z}^2) \otimes \mathbb{C}^Q$ the projection on the second component of the doubled space, we have the identity

$$\psi = \pi_2(0 \oplus \psi) = \sum_{\gamma \in \mathbb{Z}^2} \sum_{r=1}^2 \left\langle \tau_{\epsilon, \gamma} (\pi_2 F_r^{(\epsilon)}), \psi \right\rangle_{\ell^2(\mathbb{Z}^2) \otimes \mathbb{C}^Q} \left(\tau_{\epsilon, \gamma} (\pi_2 F_r^{(\epsilon)}) \right).$$

In other words this means that

$$\mathfrak{P}_2^{(\epsilon)} = \sum_{\gamma \in \mathbb{Z}^2} \sum_{r=1}^2 \left| \tau_{\epsilon, \gamma}(\pi_2 F_r^{(\epsilon)}) \right\rangle \left\langle \tau_{\epsilon, \gamma}(\pi_2 F_r^{(\epsilon)}) \right|. \quad (5.9.22)$$

The next important step consists of the following estimate that we state as a lemma.

Lemma 5.9.5. *There exist constants $\epsilon_0, \alpha, C > 0$ such that for every $0 \leq \epsilon \leq \epsilon_0$ it holds that*

$$\left| \Pi_2^{(\epsilon)}(\gamma, \underline{x}; \gamma', \underline{x}') - T_2^{(\epsilon)}(\gamma, \underline{x}; \gamma', \underline{x}') \right| \leq C \epsilon e^{-\alpha \|\gamma - \gamma'\|}. \quad (5.9.23)$$

Proof. Considering the fact that $\Pi_2^{(\epsilon)}$ is defined as in (5.9.18) and the equalities (5.9.9) and (5.9.19) hold, we have

$$\begin{aligned} & \left| \Pi_2^{(\epsilon)}(\gamma, \underline{x}; \gamma', \underline{x}') - T_2^{(\epsilon)}(\gamma, \underline{x}; \gamma', \underline{x}') \right| \\ & \leq \left| \Pi^{(\epsilon)}(\gamma, \underline{x}; \gamma', \underline{x}') - \widehat{\Pi}^{(\epsilon)}(\gamma, \underline{x}; \gamma', \underline{x}') \right| \\ & \quad + \left| \Pi_1^{(\epsilon)}(\gamma, \underline{x}; \gamma', \underline{x}') - \widehat{\Pi}_1^{(\epsilon)}(\gamma, \underline{x}; \gamma', \underline{x}') \right| \\ & \leq C \epsilon e^{-\alpha \|\gamma - \gamma'\|} + \left| \Pi_1^{(\epsilon)}(\gamma, \underline{x}; \gamma', \underline{x}') - \widehat{\Pi}_1^{(\epsilon)}(\gamma, \underline{x}; \gamma', \underline{x}') \right|, \end{aligned}$$

which is a consequence of the estimate (5.8.5). Therefore it suffices to prove that the matrix elements of $\Pi_1^{(\epsilon)} - \widehat{\Pi}_1^{(\epsilon)}$ are exponentially localized and proportional to ϵ . Since we have proved that this is true for the difference $\widetilde{\Pi}_1^{(\epsilon)} - \widehat{\Pi}_1^{(\epsilon)}$, where $\widetilde{\Pi}_1^{(\epsilon)}$ is defined in (5.9.10) (see (5.9.12)), it suffices to prove the required estimate on the matrix elements of the difference $\Pi_1^{(\epsilon)} - \widetilde{\Pi}_1^{(\epsilon)}$. Since the $(\gamma, \underline{x}; \gamma', \underline{x}')$ -matrix element of this difference is provided by a difference of absolutely convergent series, we can estimate

$$\begin{aligned} & \left| \Pi_1^{(\epsilon)}(\gamma, \underline{x}; \gamma', \underline{x}') - \widetilde{\Pi}_1^{(\epsilon)}(\gamma, \underline{x}; \gamma', \underline{x}') \right| \\ & = \left| \sum_{\eta \in \mathbb{Z}^2} \sum_{s=1}^{m-1} [\tau_{\epsilon, \eta} w_s^{(\epsilon)}](\gamma, \underline{x}) \overline{[\tau_{\epsilon, \eta} w_s^{(\epsilon)}](\gamma', \underline{x}')} - [\tau_{\epsilon, \eta} w_s](\gamma, \underline{x}) \overline{[\tau_{\epsilon, \eta} w_s](\gamma', \underline{x}')} \right| \\ & \leq \sum_{\eta \in \mathbb{Z}^2} \sum_{s=1}^{m-1} \left\{ \left| [\tau_{\epsilon, \eta} w_s^{(\epsilon)}](\gamma, \underline{x}) - [\tau_{\epsilon, \eta} w_s](\gamma, \underline{x}) \right| \left| [\tau_{\epsilon, \eta} w_s^{(\epsilon)}](\gamma', \underline{x}') \right| \right. \\ & \quad \left. + \left| [\tau_{\epsilon, \eta} w_s](\gamma, \underline{x}) \right| \left| [\tau_{\epsilon, \eta} w_s^{(\epsilon)}](\gamma', \underline{x}') - [\tau_{\epsilon, \eta} w_s](\gamma', \underline{x}') \right| \right\}. \end{aligned}$$

In view of (5.9.17) and of the exponential localization (5.9.3) and (5.9.16) of w_s and $w_s^{(\epsilon)}$, the conclusion follows. \square

Coupling (5.9.23) with (5.9.21) we obtain

$$\left| \Pi_2^{(\epsilon)}(\gamma, \underline{x}; \gamma', \underline{x}') - \mathfrak{P}_2^{(\epsilon)}(\gamma, \underline{x}; \gamma', \underline{x}') \right| \leq C \epsilon e^{-\alpha \|\gamma - \gamma'\|}.$$

Then, if ϵ is small enough, the above implies that the two projections $\Pi_2^{(\epsilon)}$ and $\mathfrak{P}_2^{(\epsilon)}$ are unitarily equivalent through a Kato–Nagy unitary K_ϵ given as in (5.8.10), i.e.

$\Pi_2^{(\epsilon)} = K_\epsilon \mathfrak{P}_2^{(\epsilon)} K_\epsilon^{-1}$. Therefore we have the following proposition that concludes the construction of $\Pi_2^{(\epsilon)}$.

Proposition 5.9.6. *There exist two exponentially localized functions $W_r^{(\epsilon)}$, $r \in \{1, 2\}$, such that*

$$\Pi_2^{(\epsilon)} = \sum_{\gamma \in \mathbb{Z}^2} \sum_{r=1}^2 \left| \tau_{\epsilon, \gamma} W_r^{(\epsilon)} \right\rangle \left\langle \tau_{\epsilon, \gamma} W_r^{(\epsilon)} \right|.$$

Proof. By hypothesis $\Pi^{(\epsilon)}$ commutes with the magnetic translations and by construction also $\Pi_1^{(\epsilon)}$ does; it follows that so does $\Pi_2^{(\epsilon)}$ by (5.9.18). From (5.9.22), it is also clear that $\mathfrak{P}_2^{(\epsilon)}$ commutes with the magnetic translations, and by (5.8.10) so does the Kato-Nagy unitary K_ϵ . Setting $W_r := K_\epsilon(\pi_2 F_r^{(\epsilon)})$, $r \in \{1, 2\}$ (compare (5.9.22)), the proof is concluded like that of Lemma 5.8.4. \square

Remark 5.9.7. The results presented in this section can be extended with not much effort to continuous families of magnetic Fermi-like projections $\Pi^{(\epsilon)}$ acting in $L^2(\mathbb{R}^2) \otimes \mathcal{H}$, where $\mathcal{H} = L^2((0, 1)^2)$. However, in order to apply the construction of the Parseval frames in the framework of continuous magnetic Schrödinger operators with constant magnetic field, it is necessary to prove an analogue of Proposition 5.8.3. In the continuous case the situation is more complicated and one has to fully exploit magnetic perturbation theory [87, 29, 32] (see also Appendix 2.5.2) and use some involved technical results regarding elliptic regularity and Agmon–Combes–Thomas uniform exponential decay estimates, see [37] and Appendix A.1.

Appendix A

Technical results

A.1 Combes–Thomas estimates and regularity of the kernels

The joint continuity and exponential localization of functions of the resolvent operator and of the Fermi projection integral kernel is a well-known fact and many proofs of it are scattered through the literature, amongst which we cite [104] and [19]. For the convenience of the reader and the self-consistency of the thesis, we provide in this section a short proof based on the techniques presented in [37]. We first review, in the two dimensional setting, the regularity results presented in [37]. In cases where possible we tried to improve some estimates. In the last part of the section we provide a proof of the joint continuity of the Fermi projection under the general Assumption 1.3.3. We warn the reader that the strategy and techniques used in the first and second part of this section are the same.

Consider the Hamiltonian defined in (2.2.1) and set $H_b = H$, moreover we drop the factor $\frac{1}{2}$ in front of the Laplacian. Define $-\Delta_A = H - V$. Consider the potential V , due to Assumption (1.3.2) we have that $\mathcal{D}(H) = \mathcal{D}(-\Delta_A) = H_A^2(\mathbb{R}^2)$, namely the second magnetic Sobolev space defined by

$$H_A^2(\mathbb{R}^2) = \left\{ f \in L^2(\mathbb{R}^2) \mid -\Delta_A f \in L^2(\mathbb{R}^2) \right\},$$

moreover the infinitesimally Kato smallness of V with respect to H implies

$$\inf_{z \in \rho(H_A)} \left\| V(H - z)^{-1} \right\| = 0.$$

Let us start with some preliminary results.

Proposition A.1.1. *Assume that $z \in D_\eta := \{z \in \mathbb{C} \mid \text{dist}(z, \sigma(H)) > \eta > 0\}$. Then for $i \in \{1, 2, 3\}$ there exists a constant C such that*

$$\sup_{z \in D_\eta} \langle |z| \rangle^{-1} \left\| (\mathbf{P}_A)_i (H - z)^{-1} \right\| \leq \frac{C}{\eta}. \quad (\text{A.1.1})$$

Proof. Consider $\lambda \in \mathbb{R}$, for every $\psi \in L^2(\mathbb{R}^2)$, $\|\psi\| = 1$, we have

$$\begin{aligned} & \sum_{i=1}^2 \left\| (\mathbf{P}_A)_i (-\Delta_A - i\lambda)^{-1} \psi \right\|^2 \\ &= \Re \left(\langle (-\Delta_A - i\lambda)^{-1} \psi, \psi \rangle \right) + \Re(z) \| (-\Delta_A - i\lambda)^{-1} \|^2 \\ &\leq \frac{1}{|\lambda|} + \frac{\max \Re(z), 0}{|\lambda|^2}. \end{aligned}$$

Since V is bounded we have

$$\|V(H - i\lambda)^{-1}\| \leq \frac{C}{|\lambda|}. \quad (\text{A.1.2})$$

By using the resolvent identity

$$(H - z)^{-1} = (H - i\lambda)^{-1} + (z - i\lambda)(H - i\lambda)^{-1}(H - z)^{-1}$$

together with (A.1.2) we get

$$\|(-\Delta_A - i\lambda)(H - z)^{-1}\| \leq C(\lambda, \eta)(1 + |z|). \quad (\text{A.1.3})$$

Therefore, writing

$$\|(\mathbf{P}_A)_i (H - z)^{-1}\| \leq \|(\mathbf{P}_A)_i (-\Delta_A - i\lambda)^{-1}\| \|(-\Delta_A - i\lambda)(H - z)^{-1}\|$$

we obtain the estimate (A.1.1). \square

The next step to prove the joint continuity is the so called Combes–Thomas estimate. Even if one can find a lot of proofs of this estimate in the literature, [26, 86, 37], we recall here the proof due to its crucial importance for our results. Note that we are interested in uniform estimates with respect to $z \in D_\eta$.

Proposition A.1.2 (Combes–Thomas estimate). *Assume that $z \in D_\eta$ where*

$$D_\eta := \{z \in \mathbb{C} \mid \text{dist}(z, \sigma(H)) > \eta > 0\}.$$

Denote by $r := \langle |z| \rangle$. Then there exist a δ_0 and a constant C such that for every $0 \leq \delta \leq \delta_0$ we have

$$\sup_{z \in D_\eta} \sup_{\mathbf{x}_0 \in \mathbb{R}^2} \left\| e^{\pm \frac{\delta}{r} \langle \cdot - \mathbf{x}_0 \rangle} (H - z)^{-1} e^{\mp \frac{\delta}{r} \langle \cdot - \mathbf{x}_0 \rangle} \right\| \leq \frac{C}{\eta}, \quad (\text{A.1.4})$$

$$\sup_{z \in D_\eta} \sup_{\mathbf{x}_0 \in \mathbb{R}^2} \left\{ r^{-1} \left\| (\mathbf{P}_A)_i e^{\pm \frac{\delta}{r} \langle \cdot - \mathbf{x}_0 \rangle} (H - z)^{-1} e^{\mp \frac{\delta}{r} \langle \cdot - \mathbf{x}_0 \rangle} \right\| \right\} \leq \frac{C}{\eta}. \quad (\text{A.1.5})$$

Proof. For $s \in \mathbb{R}$ the well-known Combes–Thomas rotation gives

$$e^{s \langle \cdot - \mathbf{x}_0 \rangle} (H - z) e^{-s \langle \cdot - \mathbf{x}_0 \rangle} = H - z + s \sum_{i=1}^2 w_i (\mathbf{P}_A)_i + sW_1 + s^2W_2$$

where w_i , W_1 and W_2 are bounded functions uniformly in \mathbf{x}_0 . Consider now $s = \frac{\delta}{r}$, using (A.1.1) and taking δ small enough, we obtain

$$\begin{aligned} & \sup_{z \in D_\eta} \sup_{x_0 \in \mathbb{R}^2} \left\| \left[s \sum_{i=1}^2 w_i(\mathbf{P}_A)_i + sW_1 + s^2W_2 \right] (H - z)^{-1} \right\| \\ & \leq |\delta|C \left(\frac{1}{\eta} + \frac{1}{r\eta} + \frac{|\delta|}{r^2\eta} \right) \leq \frac{1}{2}. \end{aligned}$$

Therefore we have

$$\begin{aligned} & e^{s\langle \cdot, -\mathbf{x}_0 \rangle} (H - z)^{-1} e^{-s\langle \cdot, -\mathbf{x}_0 \rangle} \\ & = (H - z)^{-1} \left\{ 1 + \left[s \sum_{i=1}^2 w_i(\mathbf{P}_A)_i + sW_1 + s^2W_2 \right] (H - z)^{-1} \right\}^{-1}. \end{aligned} \quad (\text{A.1.6})$$

which implies (A.1.4) and together with (A.1.1) we also obtain the proof of (A.1.5). \square

Remark A.1.3. Note that the constant C in Proposition A.1.2 remains bounded as $\eta \rightarrow 0$, therefore the estimates fail when z approaches the spectrum of H .

Consider now $\lambda_0 \geq 0$ large enough. Firstly notice that for $\lambda \geq \lambda_0$, estimates similar to (A.1.2) and (A.1) hold true, namely

$$\|V(H + \lambda)^{-1}\| \leq \frac{C}{\sqrt{\lambda_0}},$$

and

$$\|(\mathbf{P}_A)_i (-\Delta_A + \lambda)^{-1}\| \leq \frac{1}{\sqrt{\lambda}}.$$

Therefore, by using the resolvent identity, we obtain

$$\|(\mathbf{P}_A)_i (H + \lambda)^{-1}\| \leq \frac{1}{\sqrt{\lambda}}. \quad (\text{A.1.7})$$

By using again the resolvent identity, (A.1.6) and the previous two estimates, we get

$$\begin{aligned} & \sup_{\lambda \geq \lambda_0} \left\| (-\Delta_A + \lambda) e^{s\langle \cdot, -\mathbf{x}_0 \rangle} (H + \lambda)^{-1} e^{-s\langle \cdot, -\mathbf{x}_0 \rangle} \right\| \\ & = \sup_{\lambda \geq \lambda_0} \left\| \left(1 + V(H + \lambda)^{-1} \right) \left\{ 1 + \left[s \sum_{i=1}^2 w_i(\mathbf{P}_A)_i + sW_1 + s^2W_2 \right] (H + \lambda)^{-1} \right\}^{-1} \right\| \\ & \leq \frac{C}{\sqrt{\lambda_0}}. \end{aligned} \quad (\text{A.1.8})$$

By commuting twice we have

$$\begin{aligned} (-\Delta_A + \lambda) e^{s\langle \cdot, -\mathbf{x}_0 \rangle} & = e^{s\langle \cdot, -\mathbf{x}_0 \rangle} (-\Delta_A + \lambda) + \sum_{i=1}^2 \left[(-i\nabla)_i, e^{s\langle \cdot, -\mathbf{x}_0 \rangle} \right] (\mathbf{P}_A)_i \\ & \quad + \sum_{i=1}^2 \left[(-i\nabla)_i, \left[(-i\nabla)_i, e^{s\langle \cdot, -\mathbf{x}_0 \rangle} \right] \right] (\mathbf{P}_A)_i. \end{aligned}$$

Since $\left[(-i\nabla)_i, e^{s\langle \cdot - \mathbf{x}_0 \rangle}\right] = -is\partial_i \langle \mathbf{x} - \mathbf{x}_0 \rangle e^{s\langle \cdot - \mathbf{x}_0 \rangle}$, setting $s = \frac{c}{\sqrt{\lambda}}$ and using (A.1.8), (A.1.7) we obtain

$$\sup_{\lambda \geq \lambda_0} \left\| e^{\pm \frac{c}{\sqrt{\lambda}} \langle \cdot - \mathbf{x}_0 \rangle} (-\Delta_A + \lambda) (H + \lambda)^{-1} e^{\mp \frac{c}{\sqrt{\lambda}} \langle \cdot - \mathbf{x}_0 \rangle} \right\| \leq C(\lambda_0). \quad (\text{A.1.9})$$

Let us now prove that for N large enough the integral kernel of $(H_b - z)^{-N}$ is jointly continuous.

Consider now $\lambda > 0$ large enough, it is a well-known fact that the resolvent of the Laplacian in dimension $d = 2$ is smooth away from the diagonal and has a logarithmic singularity on the diagonal. By using the diamagnetic inequality, see for example [104, 19], one can conclude that

$$\left| (-\Delta_A + \lambda)^{-1}(\mathbf{x}; \mathbf{x}') \right| \leq (-\Delta + \lambda)^{-1}(\mathbf{x}; \mathbf{x}') \leq C e^{-\sqrt{\lambda} \|\mathbf{x} - \mathbf{x}'\|} (2 + \ln \|\mathbf{x} - \mathbf{x}'\|). \quad (\text{A.1.10})$$

We are now ready to extract from the L^2 Combes–Thomas estimate an L^2 to L^∞ estimate. Let us see more precisely how it works. From the explicit estimate (A.1.10), we deduce that there exists a constant $c \in \mathbb{R}$ such that

$$\sup_{\mathbf{x}_0 \in \mathbb{R}^2} \left\| e^{\mp c\sqrt{\lambda} \langle \cdot - \mathbf{x}_0 \rangle} (-\Delta_A + \lambda)^{-1} e^{\pm c\sqrt{\lambda} \langle \cdot - \mathbf{x}_0 \rangle} \right\|_{\mathcal{B}(L^2, L^\infty)} < \infty.$$

This, together with the L^2 estimate (A.1.9), implies

$$\begin{aligned} & \sup_{\mathbf{x}_0 \in \mathbb{R}^2} \left\| e^{\pm c\sqrt{\lambda} \langle \cdot - \mathbf{x}_0 \rangle} (H + \lambda)^{-1} e^{\mp c\sqrt{\lambda} \langle \cdot - \mathbf{x}_0 \rangle} \right\|_{\mathcal{B}(L^2, L^\infty)} \\ & \leq \sup_{\mathbf{x}_0 \in \mathbb{R}^2} \left\| e^{\pm c\sqrt{\lambda} \langle \cdot - \mathbf{x}_0 \rangle} (-\Delta_A + \lambda)^{-1} e^{\mp c\sqrt{\lambda} \langle \cdot - \mathbf{x}_0 \rangle} \right\|_{\mathcal{B}(L^2, L^\infty)} \\ & \quad \cdot \sup_{\mathbf{x}_0 \in \mathbb{R}^2} \left\| e^{\pm c\sqrt{\lambda} \langle \cdot - \mathbf{x}_0 \rangle} (-\Delta_A + \lambda) (H + \lambda)^{-1} e^{\mp c\sqrt{\lambda} \langle \cdot - \mathbf{x}_0 \rangle} \right\|_{\mathcal{B}(L^2, L^2)}, \end{aligned} \quad (\text{A.1.11})$$

where we define $\|A\|_{\mathcal{B}(L^2, L^2)}$ to be the norm of the operator $A : L^2(\mathbb{R}^2) \rightarrow L^2(\mathbb{R}^2)$. Therefore, the operator $e^{\pm c\sqrt{\lambda} \langle \cdot - \mathbf{x}_0 \rangle} (H + \lambda)^{-1} e^{\mp c\sqrt{\lambda} \langle \cdot - \mathbf{x}_0 \rangle}$ is bounded from $L^2(\mathbb{R}^2)$ to $L^\infty(\mathbb{R}^2)$ and it is a *Carleman integral operator*, see for example [104, Corollary A.1.2].

Since

$$(H + \lambda)^{-1} : L^2(\mathbb{R}^2) \rightarrow H_A^2(\mathbb{R}^2)$$

and in view of the Assumption on the magnetic potential, we have that $H_{A,loc}^2(\mathbb{R}^2) = H_{loc}^2(\mathbb{R}^2) \subset C(\mathbb{R}^2)$ via Sobolev embedding. Therefore, for $\varphi \in \mathcal{C}_0^\infty(\mathbb{R}^2)$, the function

$$\left(e^{\pm c\sqrt{\lambda} \langle \cdot - \mathbf{x}_0 \rangle} (H + \lambda)^{-1} e^{\mp c\sqrt{\lambda} \langle \cdot - \mathbf{x}_0 \rangle} \varphi \right) (\mathbf{x})$$

is continuous and it makes sense to evaluate it at the point \mathbf{x}_0 , that is

$$\int_{\mathbb{R}^2} d\mathbf{y} (H + \lambda)^{-1}(\mathbf{x}_0; \mathbf{y}) e^{c\sqrt{\lambda} \langle \mathbf{y} - \mathbf{x}_0 \rangle} \varphi(\mathbf{y}). \quad (\text{A.1.12})$$

In view of (A.1.9), equation (A.1.12) defines a bounded linear functional and can be extended to the whole Hilbert space. After that, by applying the Riesz representation theorem, we obtain that

$$\begin{aligned} & \sup_{\mathbf{x}_0 \in \mathbb{R}^2} \left\| (H + \lambda)^{-1} (\mathbf{x}_0; \cdot) e^{c\sqrt{\lambda} \langle \cdot - \mathbf{x}_0 \rangle} \right\|_{L^2(\mathbb{R}^2)} \\ &= \sup_{\mathbf{x}_0 \in \mathbb{R}^2} \left\| e^{c\sqrt{\lambda} \langle \cdot - \mathbf{x}_0 \rangle} (H + \lambda)^{-1} (\cdot; \mathbf{x}_0) \right\|_{L^2(\mathbb{R}^2)} \leq C, \end{aligned} \quad (\text{A.1.13})$$

where in the last equality we used the selfadjointness of H . Consider now the integral kernel of $(H + \lambda)^{-2}$, which is a priori defined using the integral kernel of the resolvent. From (A.1.13), the Cauchy-Schwarz inequality and the triangle inequality, we get that

$$\begin{aligned} & \sup_{\mathbf{x}, \mathbf{x}' \in \mathbb{R}^2} \left| e^{c\sqrt{\lambda} \|\mathbf{x} - \mathbf{x}'\|} (H + \lambda)^{-2} (\mathbf{x}; \mathbf{x}') \right| \\ & \leq \sup_{\mathbf{x}, \mathbf{x}' \in \mathbb{R}^2} \int_{\mathbb{R}^2} d\tilde{\mathbf{x}} e^{c\sqrt{\lambda} \langle \tilde{\mathbf{x}} - \mathbf{x} \rangle} \left| (H + \lambda)^{-1} (\mathbf{x}; \tilde{\mathbf{x}}) \right| \left| (H + \lambda)^{-1} (\tilde{\mathbf{x}}; \mathbf{x}') \right| e^{c\sqrt{\lambda} \langle \tilde{\mathbf{x}} - \mathbf{x}' \rangle} \\ & \leq \sup_{\mathbf{x} \in \mathbb{R}^2} \left\| (H + \lambda)^{-1} (\mathbf{x}; \cdot) e^{c\sqrt{\lambda} \langle \cdot - \mathbf{x} \rangle} \right\|_{L^2(\mathbb{R}^2)} \\ & \quad \cdot \sup_{\mathbf{x}' \in \mathbb{R}^2} \left\| e^{c\sqrt{\lambda} \langle \cdot - \mathbf{x}' \rangle} (H + \lambda)^{-1} (\cdot; \mathbf{x}') \right\|_{L^2(\mathbb{R}^2)} \leq C. \end{aligned} \quad (\text{A.1.14})$$

Hence we have obtained the desired L^∞ estimate, namely

$$\left| (H + \lambda)^{-2} (\mathbf{x}; \mathbf{x}') \right| \leq C e^{-c\sqrt{\lambda} \|\mathbf{x} - \mathbf{x}'\|}. \quad (\text{A.1.15})$$

Let us study how the estimate (A.1.15) propagates in the resolvent set. The strategy is the same as before. Indeed, consider $z \in D_\eta$ and from the resolvent identity we obtain

$$(H - z)^{-1} = (H + \lambda)^{-1} + (z - \lambda) (H + \lambda)^{-1} (H - z)^{-1}.$$

From (A.1.13) for every $\varphi \in L^2(\mathbb{R}^2)$ we get

$$\begin{aligned} & \sup_{\mathbf{x}_0 \in \mathbb{R}^2} \sup_{\mathbf{x} \in \mathbb{R}^2} \left| \int_{\mathbb{R}^2} d\tilde{\mathbf{x}} e^{-\frac{\delta}{r} \langle \mathbf{x} - \mathbf{x}_0 \rangle} (H + \lambda)^{-1} (\mathbf{x}; \tilde{\mathbf{x}}) e^{\frac{\delta}{r} \langle \tilde{\mathbf{x}} - \mathbf{x}_0 \rangle} \varphi(\tilde{\mathbf{x}}) \right| \\ & \leq \sup_{\mathbf{x}_0 \in \mathbb{R}^2} \sup_{\mathbf{x} \in \mathbb{R}^2} \int_{\mathbb{R}^2} d\tilde{\mathbf{x}} \left| (H + \lambda)^{-1} (\mathbf{x}; \tilde{\mathbf{x}}) \right| e^{c\sqrt{\lambda} \langle \tilde{\mathbf{x}} - \mathbf{x} \rangle} \varphi(\tilde{\mathbf{x}}) \\ & \leq \sup_{\mathbf{x}_0 \in \mathbb{R}^2} \sup_{\mathbf{x} \in \mathbb{R}^2} \left\| (H + \lambda)^{-1} (\mathbf{x}; \cdot) e^{c\sqrt{\lambda} \langle \cdot - \mathbf{x} \rangle} \right\|_{L^2(\mathbb{R}^2)} \|\varphi\|_{L^2(\mathbb{R}^2)}. \end{aligned}$$

Hence

$$\sup_{\mathbf{x}_0 \in \mathbb{R}^2} \left\| e^{-\frac{\delta}{r} \langle \cdot - \mathbf{x}_0 \rangle} (H + \lambda)^{-1} e^{\frac{\delta}{r} \langle \cdot - \mathbf{x}_0 \rangle} \right\|_{\mathcal{B}(L^2, L^\infty)} \leq C.$$

This, together with the L^2 bound (A.1.4) and the resolvent identity, implies that

$$\begin{aligned}
& \sup_{\mathbf{x}_0 \in \mathbb{R}^2} \left\| e^{-\frac{\delta}{r} \langle \cdot, -\mathbf{x}_0 \rangle} (H - z)^{-1} e^{\frac{\delta}{r} \langle \cdot, -\mathbf{x}_0 \rangle} \right\|_{\mathcal{B}(L^2, L^\infty)} \\
& \leq \sup_{\mathbf{x}_0 \in \mathbb{R}^2} \left\| e^{-\frac{\delta}{r} \langle \cdot, -\mathbf{x}_0 \rangle} (H + \lambda)^{-1} e^{\frac{\delta}{r} \langle \cdot, -\mathbf{x}_0 \rangle} \right\|_{\mathcal{B}(L^2, L^\infty)} \\
& \quad + (|z| + |\lambda|) \sup_{\mathbf{x}_0 \in \mathbb{R}^2} \left\| e^{-\frac{\delta}{r} \langle \cdot, -\mathbf{x}_0 \rangle} (H + \lambda)^{-1} e^{\frac{\delta}{r} \langle \cdot, -\mathbf{x}_0 \rangle} \right\|_{\mathcal{B}(L^2, L^\infty)} \\
& \quad \cdot \sup_{\mathbf{x}_0 \in \mathbb{R}^2} \left\| e^{-\frac{\delta}{r} \langle \cdot, -\mathbf{x}_0 \rangle} (H - z)^{-1} e^{\frac{\delta}{r} \langle \cdot, -\mathbf{x}_0 \rangle} \right\|_{\mathcal{B}(L^2, L^2)} \\
& \leq C \frac{r}{\eta}.
\end{aligned} \tag{A.1.16}$$

Therefore, for every function $\varphi \in C_0^\infty(\mathbb{R}^2)$, we can consider the linear functional

$$\int_{\mathbb{R}^2} d\mathbf{y} (H - z)^{-1}(\mathbf{x}_0; \mathbf{y}) e^{\frac{\delta}{r} \langle \mathbf{y}, -\mathbf{x}_0 \rangle} \varphi(\mathbf{y}) \tag{A.1.17}$$

which, considering the estimate in equation (A.1.16), defines a bounded linear functional and can be extended to the whole Hilbert space. Then, by using the Riesz representation theorem, we obtain that

$$\begin{aligned}
& \sup_{\mathbf{x}_0 \in \mathbb{R}^2} \left\| (H - z)^{-1}(\mathbf{x}_0; \cdot) e^{\frac{\delta}{r} \langle \cdot, -\mathbf{x}_0 \rangle} \right\|_{L^2(\mathbb{R}^2)} \\
& = \sup_{\mathbf{x}_0 \in \mathbb{R}^2} \left\| (H - \bar{z})^{-1}(\cdot; \mathbf{x}_0) e^{\frac{\delta}{r} \langle \cdot, -\mathbf{x}_0 \rangle} \right\|_{L^2(\mathbb{R}^2)} \leq C \frac{r}{\eta}.
\end{aligned} \tag{A.1.18}$$

Thus we have

$$\begin{aligned}
& \sup_{\mathbf{x}, \mathbf{x}' \in \mathbb{R}^2} \left| e^{\frac{\delta}{r} |\mathbf{x} - \mathbf{x}'|} (H - z)^{-2}(\mathbf{x}; \mathbf{x}') \right| \\
& \leq \sup_{\mathbf{x}, \mathbf{x}' \in \mathbb{R}^2} \int_{\mathbb{R}^2} d\tilde{\mathbf{x}} e^{\frac{\delta}{r} \langle \tilde{\mathbf{x}}, -\mathbf{x} \rangle} \left| (H - z)^{-1}(\mathbf{x}; \tilde{\mathbf{x}}) \right| \left| (H - z)^{-1}(\tilde{\mathbf{x}}; \mathbf{x}') \right| e^{\frac{\delta}{r} \langle \tilde{\mathbf{x}}, -\mathbf{x}' \rangle} \\
& \leq \sup_{\mathbf{x} \in \mathbb{R}^2} \left\| (H - z)^{-1}(\mathbf{x}; \cdot) e^{\frac{\delta}{r} \langle \cdot, -\mathbf{x} \rangle} \right\|_{L^2(\mathbb{R}^2)} \\
& \quad \sup_{\mathbf{x}' \in \mathbb{R}^2} \left\| e^{\frac{\delta}{r} \langle \cdot, -\mathbf{x}' \rangle} (H - z)^{-1}(\cdot; \mathbf{x}') \right\|_{L^2(\mathbb{R}^2)} \leq C \frac{r^2}{\eta^2}.
\end{aligned} \tag{A.1.19}$$

By a simple induction argument, we can easily conclude that

$$\left| (H - z)^{-N}(\mathbf{x}; \mathbf{x}') \right| \leq C \frac{r^N}{\eta^N} e^{-\frac{\delta}{r} \|\mathbf{x} - \mathbf{x}'\|}. \tag{A.1.20}$$

Indeed, choosing $\delta' < \delta$, we obtain

$$\begin{aligned}
 & \sup_{\mathbf{x}, \mathbf{x}' \in \mathbb{R}^2} \left| e^{\frac{\delta'}{r} |\mathbf{x} - \mathbf{x}'|} (H - z)^{-(N+1)} (\mathbf{x}; \mathbf{x}') \right| \\
 & \leq \sup_{\mathbf{x}, \mathbf{x}' \in \mathbb{R}^2} \int_{\mathbb{R}^2} d\tilde{\mathbf{x}} e^{\frac{\delta'}{r} (\tilde{\mathbf{x}} - \mathbf{x})} \left| (H - z)^{-1} (\mathbf{x}; \tilde{\mathbf{x}}) \right| \left| (H - z)^{-N} (\tilde{\mathbf{x}}; \mathbf{x}') \right| e^{\frac{\delta'}{r} (\tilde{\mathbf{x}} - \mathbf{x}')} \\
 & \leq C \frac{r^N}{\eta^N} \sup_{\mathbf{x}, \mathbf{x}' \in \mathbb{R}^2} \int_{\mathbb{R}^2} d\tilde{\mathbf{x}} e^{\frac{\delta}{r} (\tilde{\mathbf{x}} - \mathbf{x})} \left| (H - z)^{-1} (\mathbf{x}; \tilde{\mathbf{x}}) \right| e^{-(\delta - \delta') \|\tilde{\mathbf{x}} - \mathbf{x}'\|} \\
 & \leq C \frac{r^N}{\eta^N} \sup_{\mathbf{x} \in \mathbb{R}^2} \left\| e^{\frac{\delta}{r} \langle \cdot - \mathbf{x} \rangle} (H - z)^{-1} (\mathbf{x}; \cdot) \right\|_{L^2(\mathbb{R}^2)} \left\| e^{-(\delta - \delta') \|\cdot - \mathbf{x}'\|} \right\|_{L^2(\mathbb{R}^2)} \\
 & \leq C \frac{r^{N+1}}{\eta^{N+1}}.
 \end{aligned}$$

However, the estimate (A.1.20) is not optimal and we can do something better. Consider $N > 1$. By using (A.1.16) and the Combes–Thomas estimate (A.1.4), we obtain

$$\begin{aligned}
 & \sup_{\mathbf{x}_0 \in \mathbb{R}^2} \left\| e^{-\frac{\delta}{r} \langle \cdot - \mathbf{x}_0 \rangle} (H - z)^{-N} e^{\frac{\delta}{r} \langle \cdot - \mathbf{x}_0 \rangle} \right\|_{\mathcal{B}(L^2, L^\infty)} \\
 & \leq \sup_{\mathbf{x}_0 \in \mathbb{R}^2} \left\| e^{-\frac{\delta}{r} \langle \cdot - \mathbf{x}_0 \rangle} (H - z)^{-1} e^{\frac{\delta}{r} \langle \cdot - \mathbf{x}_0 \rangle} \right\|_{\mathcal{B}(L^2, L^\infty)} \\
 & \quad \cdot \sup_{\mathbf{x}_0 \in \mathbb{R}^2} \left\| e^{-\frac{\delta}{r} \langle \cdot - \mathbf{x}_0 \rangle} (H - z)^{-(N-1)} e^{\frac{\delta}{r} \langle \cdot - \mathbf{x}_0 \rangle} \right\|_{\mathcal{B}(L^2, L^2)} \\
 & \leq C \frac{r}{\eta^N},
 \end{aligned} \tag{A.1.21}$$

from which we get

$$\begin{aligned}
 & \sup_{\mathbf{x}_0 \in \mathbb{R}^2} \left\| (H - z)^{-N} (\mathbf{x}_0; \cdot) e^{\frac{\delta}{r} \langle \cdot - \mathbf{x}_0 \rangle} \right\|_{L^2(\mathbb{R}^2)} \\
 & = \sup_{\mathbf{x}_0 \in \mathbb{R}^2} \left\| (H - \bar{z})^{-N} (\cdot; \mathbf{x}_0) e^{\frac{\delta}{r} \langle \cdot - \mathbf{x}_0 \rangle} \right\|_{L^2(\mathbb{R}^2)} \leq C \frac{r}{\eta^N}.
 \end{aligned} \tag{A.1.22}$$

Therefore, using (A.1.18) and (A.1.22), we obtain

$$\begin{aligned}
 & \sup_{\mathbf{x}, \mathbf{x}' \in \mathbb{R}^2} \left| e^{\frac{\delta'}{r} \|\mathbf{x} - \mathbf{x}'\|} (H - z)^{-N} (\mathbf{x}; \mathbf{x}') \right| \\
 & \leq \sup_{\mathbf{x}, \mathbf{x}' \in \mathbb{R}^2} \int_{\mathbb{R}^2} d\tilde{\mathbf{x}} e^{\frac{\delta'}{r} (\tilde{\mathbf{x}} - \mathbf{x})} \left| (H - z)^{-1} (\mathbf{x}; \tilde{\mathbf{x}}) \right| \left| (H - z)^{-(N-1)} (\tilde{\mathbf{x}}; \mathbf{x}') \right| e^{\frac{\delta'}{r} (\tilde{\mathbf{x}} - \mathbf{x}')} \\
 & \leq \sup_{\mathbf{x} \in \mathbb{R}^2} \left\| (H - z)^{-1} (\mathbf{x}; \cdot) e^{\frac{\delta}{r} \langle \cdot - \mathbf{x} \rangle} \right\|_{L^2(\mathbb{R}^2)} \sup_{\mathbf{x}' \in \mathbb{R}^2} \left\| e^{\frac{\delta}{r} \langle \cdot - \mathbf{x}' \rangle} (H - z)^{-(N-1)} (\cdot; \mathbf{x}') \right\|_{L^2(\mathbb{R}^2)} \\
 & \leq C \frac{r^2}{\eta^N}.
 \end{aligned} \tag{A.1.23}$$

Comparing (A.1.23) and (A.1.20), one can see that exploiting the Combes–Thomas norm estimate we managed to obtain a better estimate in terms of r . However, notice that the estimate still has a factor η^{-N} , which clearly explodes when z approaches the spectrum of H .

Let us now show that, for N large enough, we have similar estimates for the operator $(\mathbf{P}_A)_i (H - z)^{-N}$, $i \in \{1, 2\}$. Consider the identity

$$(\mathbf{P}_A)_i (H - z)^{-1} = (H - z)^{-1} (\mathbf{P}_A)_i + (H - z)^{-2} T_1,$$

where $T_1 = [H, (\mathbf{P}_A)_i] + [H, [H, (\mathbf{P}_A)_i]] (H - z)^{-1}$. Since, for $i \neq j$, $i, j \in \{1, 2\}$, the operators

$$\begin{aligned} [H, (\mathbf{P}_A)_i] &= [V, -i(\nabla)_i] = 2ib(\mathbf{P}_A)_j + i\partial_i(V), \\ [H, [H, (\mathbf{P}_A)_i]] &= -2b(2b(\mathbf{P}_A)_i + \partial_j V) \\ &\quad + \sum_{l=1}^2 -i\partial_l^2 \partial_i(V) + 2 \sum_{l=1}^2 \partial_l \partial_i(V) (\mathbf{P}_A)_j, \end{aligned}$$

are relatively bounded with respect to H , we get that T_1 is a bounded operator. This fact, together with (A.1.1) and (A.1.6), implies that

$$\sup_{\mathbf{x}_0 \in \mathbb{R}^2} \left\| e^{\pm \frac{\delta}{r} \langle \cdot - \mathbf{x}_0 \rangle} T_1 e^{\mp \frac{\delta}{r} \langle \cdot - \mathbf{x}_0 \rangle} \right\| < C \frac{r}{\eta}. \quad (\text{A.1.24})$$

Thus, by commuting twice we obtain the identity

$$(\mathbf{P}_A)_i (H - z)^{-2} = (H - z)^{-2} \left((\mathbf{P}_A)_i + (H - z)^{-1} T_1 + T_1 (H - z)^{-1} \right).$$

Therefore we have

$$\begin{aligned} (\mathbf{P}_A)_i (H - z)^{-N} &= (\mathbf{P}_A)_i (H - z)^{-2} (H - z)^{-N+2} \\ &= (H - z)^{-2} T (H - z)^{-N+5} (H - z)^{-2} \end{aligned}$$

with $T = \left((\mathbf{P}_A)_i + (H - z)^{-1} T_1 + T_1 (H - z)^{-1} \right) (H - z)^{-1}$.

The estimates (A.1.1), (A.1.4) and (A.1.24) imply that

$$\sup_{\mathbf{x}_0 \in \mathbb{R}^2} \left\| e^{\pm \frac{\delta}{r} \langle \cdot - \mathbf{x}_0 \rangle} T e^{\mp \frac{\delta}{r} \langle \cdot - \mathbf{x}_0 \rangle} \right\| < C \frac{r}{\eta}. \quad (\text{A.1.25})$$

Consider now $N > 5$, $N \in \mathbb{N}$, from (A.1.4), (A.1.25) and (A.1.16) we obtain

$$\sup_{\mathbf{x}_0 \in \mathbb{R}^2} \left\| e^{-\frac{\delta}{r} \langle \cdot - \mathbf{x}_0 \rangle} (H - z)^{-2} T (H - z)^{-N+5} e^{\frac{\delta}{r} \langle \cdot - \mathbf{x}_0 \rangle} \right\|_{\mathcal{B}(L^2, L^\infty)} \leq C \frac{r^2}{\eta^2}. \quad (\text{A.1.26})$$

Using the same procedure as before we obtain the following L^2 estimate

$$\sup_{\mathbf{x}_0 \in \mathbb{R}^2} \left\| \left((H - z)^{-2} T (H - z)^{-N+5} \right) (\mathbf{x}_0; \cdot) e^{\frac{\delta}{r} \langle \cdot - \mathbf{x}_0 \rangle} \right\|_{L^2(\mathbb{R}^2)} \leq C \frac{r^2}{\eta^2},$$

which together with (A.1.19) implies

$$\begin{aligned}
 & \sup_{\mathbf{x}, \mathbf{x}' \in \mathbb{R}^2} e^{\frac{\delta}{r} \|\mathbf{x} - \mathbf{x}'\|} \left| \left((\mathbf{P}_A)_i (H - z)^{-N} \right) (\mathbf{x}; \mathbf{x}') \right| \\
 & \leq \sup_{\mathbf{x}, \mathbf{x}' \in \mathbb{R}^2} \int_{\mathbb{R}^2} d\tilde{\mathbf{x}} e^{\frac{\delta}{r} \langle \tilde{\mathbf{x}} - \mathbf{x} \rangle} \left| \left((H - z)^{-2} T (H - z)^{-N+5} \right) (\mathbf{x}; \tilde{\mathbf{x}}) \right| \\
 & \quad \cdot \left| (H - z)^{-2} (\tilde{\mathbf{x}}; \mathbf{x}') \right| e^{\frac{\delta}{r} \langle \tilde{\mathbf{x}} - \mathbf{x}' \rangle} \\
 & \leq \sup_{\mathbf{x} \in \mathbb{R}^2} \left\| \left((H - z)^{-2} T (H - z)^{-N+5} \right) (\mathbf{x}; \cdot) e^{\frac{\delta}{r} \langle \cdot - \mathbf{x} \rangle} \right\|_{L^2(\mathbb{R}^2)} \\
 & \quad \cdot \sup_{\mathbf{x}' \in \mathbb{R}^2} \left\| e^{\frac{\delta}{r} \langle \cdot - \mathbf{x}' \rangle} (H - z)^{-2} (\cdot; \mathbf{x}') \right\|_{L^2(\mathbb{R}^2)} \\
 & \leq C \frac{r^4}{\eta^4}.
 \end{aligned} \tag{A.1.27}$$

It remains to prove the joint continuity of the integral kernels of $(\mathbf{P}_A)_i (H - z)^{-N}$ and $(H - z)^{-N}$. Let us start with $(H - z)^{-N}$. Consider an open and bounded subset $U \subset \mathbb{R}^2$ and a compactly supported function $g_U \in C^\infty$ defined by $g_U(\mathbf{x}) = 1$ for every $\mathbf{x} \in U$ and such that $|g_U(\mathbf{x})| \leq 1$ for all $\mathbf{x} \in \mathbb{R}^2$. The joint continuity of the integral kernels will follow easily if we prove the joint continuity of the operator

$$g_U (H - z)^{-N} g_U.$$

The strategy is to show that this operator has a continuous integral kernel for every U exploiting the regularizing properties of the resolvent of H . Let us show this in details. Consider the trivial identity

$$g_U (H - z)^{-N} g_U = (H - z)^{-1} (H - z) g_U (H - z)^{-N} g_U (H - z) (H - z)^{-1}.$$

We first prove that $(H - z) g_U (H - z)^{-N} g_U (H - z)$ is a Hilbert–Schmidt operator. Indeed, by commuting $(H - z)$ with the functions g_U , we get

$$\begin{aligned}
 & g_U (H - z)^{-N+2} g_U \\
 & + g_U (H - z)^{-N+2} \left((H - z)^{-1} 2i \sum_{i=1}^2 (\mathbf{P}_A)_i \partial_i g_U + (H - z)^{-1} \Delta(g_U) \right) \\
 & + \left(-2i \sum_{i=1}^2 \partial_i g_U (\mathbf{P}_A)_i (H - z)^{-1} - \Delta(g_U) (H - z)^{-1} \right) (H - z)^{-N+2} g_U \\
 & + \left(-2i \sum_{i=1}^2 \partial_i g_U (\mathbf{P}_A)_i (H - z)^{-1} - \Delta(g_U) (H - z)^{-1} \right) (H - z)^{-N+2} \\
 & \quad \cdot \left((H - z)^{-1} 2i \sum_{i=1}^2 (\mathbf{P}_A)_i \partial_i g_U + (H - z)^{-1} \Delta(g_U) \right).
 \end{aligned} \tag{A.1.28}$$

From (A.1.20) we have that $g_U (H - z)^{-N+2}$ and $(H - z)^{-N+2} g_U$ are Hilbert–Schmidt operators. Indeed, consider for example $g_U (H - z)^{-N+2}$, it holds that

$$\left| g_U e^{\|\cdot\|} e^{-\|\cdot\|} (H - z)^{-N+2} (\mathbf{x}; \mathbf{x}') \right| \leq \frac{C_U r^N}{\eta} e^{-\|\mathbf{x}\|} e^{-\frac{\delta}{r} \|\mathbf{x} - \mathbf{x}'\|},$$

hence its kernel is in $L^2(\mathbb{R}^2 \times \mathbb{R}^2)$. A similar argument, together with (A.1.1), shows that the first three terms of (A.1.28) are Hilbert–Schmidt operators. From (A.1.5) it is not difficult to deduce, by commuting $(\mathbf{P}_A)_i$ with the exponential weight, that

$$\left\| e^{\pm \frac{\delta}{r} \langle \cdot - \mathbf{x}_0 \rangle} (\mathbf{P}_A)_i (H - z)^{-1} e^{\mp \frac{\delta}{r} \langle \cdot - \mathbf{x}_0 \rangle} \right\| \leq C.$$

Therefore one can show that also the last term is a Hilbert–Schmidt operator, because $e^{-\frac{\delta}{r} \langle \cdot - \mathbf{x}_0 \rangle} (H - z)^{-N+2}$ is Hilbert–Schmidt and

$$\begin{aligned} & -2i \sum_{i=1}^2 \partial_i g_U e^{\frac{\delta}{r} \langle \cdot - \mathbf{x}_0 \rangle} e^{-\frac{\delta}{r} \langle \cdot - \mathbf{x}_0 \rangle} (\mathbf{P}_A)_i (H - z)^{-1} e^{\frac{\delta}{r} \langle \cdot - \mathbf{x}_0 \rangle}, \\ & \Delta(g_U) e^{\frac{\delta}{r} \langle \cdot - \mathbf{x}_0 \rangle} e^{-\frac{\delta}{r} \langle \cdot - \mathbf{x}_0 \rangle} (H - z)^{-1} e^{\frac{\delta}{r} \langle \cdot - \mathbf{x}_0 \rangle}, \end{aligned}$$

are bounded operators.

From the previous arguments it follows that the operator

$$(H - z) g_U (H - z)^{-N} g_U (H - z)$$

admits an integral kernel, call it $W(\mathbf{x}; \mathbf{x}')$. Thus W has to be in $L^2(\mathbb{R}^2 \times \mathbb{R}^2)$. By definition of tensor product of Hilbert spaces, W can be approximated in the $L^2(\mathbb{R}^2 \times \mathbb{R}^2)$ norm by a finite sum of the form

$$\sum_{j=1}^M g_j(\mathbf{x}) f_j(\mathbf{x}'),$$

with $g_j, f_j \in L^2(\mathbb{R}^2)$. This means that, by means of the Cauchy-Schwarz inequality, we get that the integral kernel of $g_U (H - z)^{-N} g_U$ can be approximated uniformly for every $\mathbf{x}, \mathbf{x}' \in U$ by

$$g_U (H - z)^{-N} g_U(\mathbf{x}; \mathbf{x}') = \lim_{M \rightarrow \infty} \sum_{j=1}^M \left((H - z)^{-1} g_j \right)(\mathbf{x}) \overline{\left((H - \bar{z})^{-1} f_j \right)(\mathbf{x}')}.$$

Explicitly we have

$$\begin{aligned} & \sup_{\mathbf{x}, \mathbf{x}' \in \mathbb{R}^2} \left| \int_{\mathbb{R}^2} d\mathbf{y} \int_{\mathbb{R}^2} d\mathbf{y}' (H - z)^{-1}(\mathbf{x}; \mathbf{y}) \right. \\ & \quad \cdot \left(W(\mathbf{y}, \mathbf{y}') - \sum_{j=1}^M g_j(\mathbf{y}) f_j(\mathbf{y}') \right) (H - z)^{-1}(\mathbf{y}'; \mathbf{x}') \left. \right| \\ & \leq \left\| W - \sum_{j=1}^M g_j f_j \right\|_{L^2(\mathbb{R}^2 \times \mathbb{R}^2)} \sup_{\mathbf{x} \in \mathbb{R}^2} \left\| (H - z)^{-1}(\mathbf{x}; \cdot) \right\|_{L^2(\mathbb{R}^2)} \\ & \quad \cdot \sup_{\mathbf{x}' \in \mathbb{R}^2} \left\| (H - z)^{-1}(\cdot; \mathbf{x}') \right\|_{L^2(\mathbb{R}^2)}. \end{aligned}$$

Since $(H - z)^{-1} : L^2(\mathbb{R}^2) \rightarrow H_A^2(\mathbb{R}^2)$, the Sobolev embedding mentioned before is enough to conclude that the integral kernel of $g_U (H - z)^{-N} g_U$ is a uniform limit of continuous functions and therefore it is a jointly continuous integral kernel.

By mimicking the previous proof, and considering that

$$\begin{aligned} & (\mathbf{P}_A)_i (H - z)^{-N} \\ &= (H - z)^{-1} (\mathbf{P}_A)_i (H - z)^{-N-1} - i (H - z)^{-1} \partial_i (V) (H - z)^{-N-1} , \end{aligned}$$

one can prove the joint continuity of the integral kernel of $(\mathbf{P}_A)_i (H - z)^{-N}$. An analogous proof shows that also Π_0 has a jointly continuous integral kernel.

A.1.1 Kernel of the Fermi projection P_μ

Let us now consider a Hamiltonian satisfying Assumption 1.3.3 and prove that the projection P_μ admits a jointly continuous integral kernel. The strategy of the proof is identical to the one used in the previous section, however one has to be more careful in handling unbounded scalar potentials. Regarding the magnetic potential, the situation is very similar to the previous one, since the hypothesis on \mathbf{A} assure that we can apply the diamagnetic inequality by means of equation (A.1.10). Moreover, the Assumption 1.3.3 on the Hamiltonian together with the Sobolev embedding assure that, also in this setting, the domain of the Hamiltonian is made of continuous functions. Indeed, since V is relatively bounded with respect to $-\Delta_A$, the domain of the Hamiltonian is given by the second magnetic Sobolev space $H_A^2(\mathbb{R}^2)$ defined using the magnetic vector potential \mathbf{A} , that is consider

$$H_A^1(\mathbb{R}^2) := \left\{ \psi \in L^2(\mathbb{R}^2) \mid (-i\nabla - \mathbf{A}) \psi \in L^2(\mathbb{R}^2, \mathbb{R}^2) \right\} ,$$

then

$$H_A^2(\mathbb{R}^2) := \left\{ \psi \in H_A^1(\mathbb{R}^2) \mid (-i\nabla - \mathbf{A})^2 \psi \in L^2(\mathbb{R}^2) \right\} .$$

Let now $\psi \in H_A^2(\mathbb{R}^2)$ and $\varphi \in C_0^\infty$. A simple computation shows that

$$(-i\nabla)_j (\varphi\psi) = -i (\partial_j \varphi) \psi + \varphi (-i\nabla - \mathbf{A})_j \psi + \varphi \mathbf{A}_j \psi \in L^2(\mathbb{R}^2)$$

because $\varphi \mathbf{A}_j \in L^2(\mathbb{R}^2)$ (since $\mathbf{A}_j \in L_{loc}^2(\mathbb{R}^2)$ by hypothesis), and

$$\varphi \mathbf{A}_j \psi = \varphi \mathbf{A}_j (-\Delta_A + i) (-\Delta_A + i)^{-1} \psi .$$

Hence $\varphi\psi \in H_A^1(\mathbb{R}^2)$. Then we have

$$(-i\nabla - \mathbf{A})^2 (\varphi\psi) = \varphi (-i\nabla - \mathbf{A})^2 \psi - (\Delta \varphi) \psi - 2i (\nabla \varphi) \cdot (-i\nabla - \mathbf{A}) \psi \in L^2(\mathbb{R}^2) .$$

Therefore $(-i\nabla - \mathbf{A})^2 (\varphi\psi) \in H_A^2(\mathbb{R}^2)$. Thus we have

$$\begin{aligned} -\Delta (\varphi\psi) &= (-i\nabla - \mathbf{A} + \mathbf{A})^2 (\varphi\psi) \\ &= (-i\nabla - \mathbf{A})^2 (\varphi\psi) + \mathbf{A}^2 (\varphi\psi) + 2\mathbf{A} \cdot (-i\nabla - \mathbf{A}) (\varphi\psi) - i\nabla \cdot \mathbf{A} (\varphi\psi) , \end{aligned}$$

which, in view of the hypothesis on \mathbf{A} , the compactness of the support of $\varphi\psi$ and the fact that $(-i\nabla - \mathbf{A})$ preserves the support of the function, implies that $\varphi\psi \in H^2(\mathbb{R}^2)$. Since we are in $d = 2$, a standard Sobolev embedding argument shows that $\varphi\psi$ is a continuous function. An opportune choice of the function φ shows that ψ is a continuous function on every compact set of \mathbb{R}^2 .

Proposition A.1.4. *Assume that $z \in D_\eta := \{z \in \mathbb{C} \mid \text{dist}(z, \sigma(H)) > \eta > 0\}$. Then for $i \in \{1, 2, 3\}$ there exists a constant C such that*

$$\sup_{z \in D_\eta} \langle |z| \rangle^{-1} \left\| (\mathbf{P}_A)_i (H - z)^{-1} \right\| \leq \frac{C}{\eta}. \quad (\text{A.1.29})$$

Proof. Consider $\lambda \in \mathbb{R}$, for every $\psi \in L^2(\mathbb{R}^2)$, $\|\psi\| = 1$, we have

$$\begin{aligned} & \sum_{i=1}^2 \left\| (\mathbf{P}_A)_i (-\Delta_A - i\lambda)^{-1} \psi \right\|^2 \\ &= \Re \left(\langle (-\Delta_A - i\lambda)^{-1} \psi, \psi \rangle \right) + \Re(z) \left\| (-\Delta_A - i\lambda)^{-1} \right\|^2 \\ &\leq \frac{1}{|\lambda|} + \frac{\max \Re(z), 0}{|\lambda|^2}. \end{aligned}$$

Since V is relatively bounded with respect to H , there exists a λ such that (see [1, Proposition 2.42])

$$\left\| V (H - i\lambda)^{-1} \right\| \leq \frac{1}{2}. \quad (\text{A.1.30})$$

By using the resolvent identity

$$(H - z)^{-1} = (H - i\lambda)^{-1} + (z - i\lambda) (H - i\lambda)^{-1} (H - z)^{-1}$$

together with (A.1.30) we get

$$\left\| (-\Delta_A - i\lambda) (H - z)^{-1} \right\| \leq C(\lambda, \eta)(1 + |z|). \quad (\text{A.1.31})$$

Therefore, writing

$$\left\| (\mathbf{P}_A)_i (H - z)^{-1} \right\| \leq \left\| (\mathbf{P}_A)_i (-\Delta_A - i\lambda)^{-1} \right\| \left\| (-\Delta_A - i\lambda) (H - z)^{-1} \right\|$$

we obtain the estimate (A.1.29). \square

By mimicking the strategy of the previous section, we prove the Combes–Thomas estimate for the resolvent in this general setting.

Proposition A.1.5 (Combes–Thomas estimate in the general setting). *Assume that $z \in K$ where K is a compact subset of D_η . Denote by $\bar{r} = \sup_{z \in K} r = \sup_{z \in K} \langle |z| \rangle$. Then there exists a δ_0 and a constant C such that for every $0 \leq \delta \leq \delta_0$ we have*

$$\sup_{z \in K} \sup_{\mathbf{x}_0 \in \mathbb{R}^2} \left\| e^{\pm \frac{\delta}{\bar{r}} \langle \cdot - \mathbf{x}_0 \rangle} (H - z)^{-1} e^{\mp \frac{\delta}{\bar{r}} \langle \cdot - \mathbf{x}_0 \rangle} \right\| \leq \frac{C}{\eta}, \quad (\text{A.1.32})$$

$$\sup_{z \in K} \sup_{\mathbf{x}_0 \in \mathbb{R}^2} \left\{ \bar{r}^{-1} \left\| (\mathbf{P}_A)_i e^{\pm \frac{\delta}{\bar{r}} \langle \cdot - \mathbf{x}_0 \rangle} (H - z)^{-1} e^{\mp \frac{\delta}{\bar{r}} \langle \cdot - \mathbf{x}_0 \rangle} \right\| \right\} \leq \frac{C}{\eta}. \quad (\text{A.1.33})$$

Proof. For $s \in \mathbb{R}$ the well-known Combes–Thomas rotation gives

$$e^{s \langle \cdot - \mathbf{x}_0 \rangle} (H - z) e^{-s \langle \cdot - \mathbf{x}_0 \rangle} = H - z + s \sum_{i=1}^2 w_i (\mathbf{P}_A)_i + sW_1 + s^2W_2$$

where w_i , W_1 and W_2 are bounded functions uniformly in \mathbf{x}_0 . Consider now $s = \frac{\delta}{r}$. Using (A.1.29) and taking δ small enough, we obtain

$$\begin{aligned} & \sup_{z \in K} \sup_{x_0 \in \mathbb{R}^2} \left\| \left[s \sum_{i=1}^2 w_i(\mathbf{P}_A)_i + sW_1 + s^2W_2 \right] (H - z)^{-1} \right\| \\ & \leq |\delta| \frac{C}{\eta} \left(1 + \frac{1}{r} + \frac{|\delta|}{r^2} \right) \leq \frac{1}{2}. \end{aligned}$$

Therefore we have

$$\begin{aligned} & e^{s\langle -\mathbf{x}_0 \rangle} (H - z)^{-1} e^{-s\langle -\mathbf{x}_0 \rangle} \\ & = (H - z)^{-1} \left\{ 1 + \left[s \sum_{i=1}^2 w_i(\mathbf{P}_A)_i + sW_1 + s^2W_2 \right] (H - z)^{-1} \right\}^{-1}. \end{aligned} \quad (\text{A.1.34})$$

which implies (A.1.32) and together with (A.1.29) we also obtain the proof of (A.1.33). \square

Consider now $\lambda \geq 0$ large enough. At the price of enlarging the compact subset K we can assume that $\lambda \in K$. From (A.1.34) we get

$$\begin{aligned} & \left\| (-\Delta_A + \lambda) e^{s\langle -\mathbf{x}_0 \rangle} (H + \lambda)^{-1} e^{-s\langle -\mathbf{x}_0 \rangle} \right\| \\ & = \left\| \left(1 + V(H + \lambda)^{-1} \right) \left\{ 1 + \left[s \sum_{i=1}^2 w_i(\mathbf{P}_A)_i + sW_1 + s^2W_2 \right] (H + \lambda)^{-1} \right\}^{-1} \right\| \\ & \leq C_\lambda, \end{aligned} \quad (\text{A.1.35})$$

where the constant C_λ depends on the λ chosen. By commuting twice we get

$$\begin{aligned} (-\Delta_A + \lambda) e^{s\langle -\mathbf{x}_0 \rangle} &= e^{s\langle -\mathbf{x}_0 \rangle} (-\Delta_A + \lambda) + \sum_{i=1}^2 \left[(-i\nabla)_i, e^{s\langle -\mathbf{x}_0 \rangle} \right] (\mathbf{P}_A)_i \\ & \quad + \sum_{i=1}^2 \left[(-i\nabla)_i, \left[(-i\nabla)_i, e^{s\langle -\mathbf{x}_0 \rangle} \right] \right] (\mathbf{P}_A)_i. \end{aligned}$$

Since $\left[(-i\nabla)_i, e^{s\langle -\mathbf{x}_0 \rangle} \right] = -is\partial_i \langle \mathbf{x} - \mathbf{x}_0 \rangle e^{s\langle -\mathbf{x}_0 \rangle}$, using (A.1.35) and setting $s = \frac{\delta}{r}$ with δ small enough we obtain

$$\left\| e^{\pm \frac{\delta}{r} \langle -\mathbf{x}_0 \rangle} (-\Delta_A + \lambda) (H + \lambda)^{-1} e^{\mp \frac{\delta}{r} \langle -\mathbf{x}_0 \rangle} \right\| \leq C_\eta (1 + \lambda). \quad (\text{A.1.36})$$

Let us now prove that for N large enough the integral kernel of $(H_b - z)^{-N}$ is jointly continuous.

Consider $\lambda > 0$ large enough. As we mentioned before, the assumptions on the magnetic vector potential \mathbf{A} are such that the diamagnetic inequality (A.1.10) holds true. Therefore, mimicking the strategy of the previous section we are ready to transform the L^2 Combes–Thomas estimate to an L^2 to L^∞ estimates. Let us see more precisely how it works. From (A.1.10), we deduce that there exists a constant c such that

$$\sup_{\mathbf{x}_0 \in \mathbb{R}^2} \left\| e^{\mp c\sqrt{\lambda} \langle -\mathbf{x}_0 \rangle} (-\Delta_A + \lambda)^{-1} e^{\pm c\sqrt{\lambda} \langle -\mathbf{x}_0 \rangle} \right\|_{\mathcal{B}(L^2, L^\infty)} < \infty.$$

This, together with the L^2 estimate (A.1.36), gives

$$\begin{aligned} & \sup_{\mathbf{x}_0 \in \mathbb{R}^2} \left\| e^{\pm c\sqrt{\lambda}\langle \cdot, -\mathbf{x}_0 \rangle} (H + \lambda)^{-1} e^{\mp c\sqrt{\lambda}\langle \cdot, -\mathbf{x}_0 \rangle} \right\|_{\mathcal{B}(L^2, L^\infty)} \\ & \leq \sup_{\mathbf{x}_0 \in \mathbb{R}^2} \left\| e^{\pm c\sqrt{\lambda}\langle \cdot, -\mathbf{x}_0 \rangle} (-\Delta_A + \lambda)^{-1} e^{\mp c\sqrt{\lambda}\langle \cdot, -\mathbf{x}_0 \rangle} \right\|_{\mathcal{B}(L^2, L^\infty)} \\ & \quad \cdot \sup_{\mathbf{x}_0 \in \mathbb{R}^2} \left\| e^{\pm c\sqrt{\lambda}\langle \cdot, -\mathbf{x}_0 \rangle} (-\Delta_A + z) (H - z)^{-1} e^{\mp c\sqrt{\lambda}\langle \cdot, -\mathbf{x}_0 \rangle} \right\|_{\mathcal{B}(L^2, L^2)}, \end{aligned} \quad (\text{A.1.37})$$

hence the operator $e^{\pm c\sqrt{\lambda}\langle \cdot, -\mathbf{x}_0 \rangle} (H + \lambda)^{-1} e^{\mp c\sqrt{\lambda}\langle \cdot, -\mathbf{x}_0 \rangle}$ is bounded from L^2 to L^∞ and it is a *Carleman integral operator*.

Since

$$(H + \lambda)^{-1} : L^2(\mathbb{R}^2) \rightarrow H_A^2(\mathbb{R}^2)$$

and in view of the Assumption on the magnetic potential, we have that $H_{A,loc}^2(\mathbb{R}^2) = H_{loc}^2(\mathbb{R}^2) \subset C(\mathbb{R}^2)$ via Sobolev embedding, therefore, for $\varphi \in \mathcal{C}_0^\infty(\mathbb{R}^2)$, the function

$$\left(e^{\pm c\sqrt{\lambda}\langle \cdot, -\mathbf{x}_0 \rangle} (H + \lambda)^{-1} e^{\mp c\sqrt{\lambda}\langle \cdot, -\mathbf{x}_0 \rangle} \varphi \right) (\mathbf{x})$$

is continuous and it makes sense to evaluate it at the point \mathbf{x}_0 , that is

$$\int_{\mathbb{R}^2} d\mathbf{y} (H + \lambda)^{-1} (\mathbf{x}_0, \mathbf{y}) e^{c\sqrt{\lambda}\langle \mathbf{y}, -\mathbf{x}_0 \rangle} \varphi(\mathbf{y}). \quad (\text{A.1.38})$$

In view of (A.1.9), equation (A.1.12) defines a bounded linear functional and can be extended to the whole Hilbert space, then via the Riesz representation theorem we obtain that

$$\begin{aligned} & \sup_{\mathbf{x}_0 \in \mathbb{R}^2} \left\| (H + \lambda)^{-1} (\mathbf{x}_0; \cdot) e^{c\sqrt{\lambda}\langle \cdot, -\mathbf{x}_0 \rangle} \right\|_{L^2(\mathbb{R}^2)} \\ & = \sup_{\mathbf{x}_0 \in \mathbb{R}^2} \left\| e^{c\sqrt{\lambda}\langle \cdot, -\mathbf{x}_0 \rangle} (H + \lambda)^{-1} (\cdot; \mathbf{x}_0) \right\|_{L^2(\mathbb{R}^2)} \leq C, \end{aligned} \quad (\text{A.1.39})$$

where in the last equality we used the selfadjointness of H . Consider now the integral kernel of $(H + \lambda)^{-2}$, which is a priori defined using the integral kernel of the resolvent. From (A.1.13), the Cauchy-Schwarz inequality and the triangle inequality, we get that

$$\begin{aligned} & \sup_{\mathbf{x}, \mathbf{x}' \in \mathbb{R}^2} \left| e^{c\sqrt{\lambda}\|\mathbf{x}-\mathbf{x}'\|} (H + \lambda)^{-2} (\mathbf{x}; \mathbf{x}') \right| \\ & \leq \sup_{\mathbf{x}, \mathbf{x}' \in \mathbb{R}^2} \int_{\mathbb{R}^2} d\tilde{\mathbf{x}} e^{c\sqrt{\lambda}\langle \tilde{\mathbf{x}}, -\mathbf{x} \rangle} \left| (H + \lambda)^{-1} (\mathbf{x}; \tilde{\mathbf{x}}) \right| \left| (H + \lambda)^{-1} (\tilde{\mathbf{x}}; \mathbf{x}') \right| e^{c\sqrt{\lambda}\langle \tilde{\mathbf{x}}, -\mathbf{x}' \rangle} \\ & \leq \sup_{\mathbf{x} \in \mathbb{R}^2} \left\| (H + \lambda)^{-1} (\mathbf{x}; \cdot) e^{c\sqrt{\lambda}\langle \cdot, -\mathbf{x} \rangle} \right\|_{L^2(\mathbb{R}^2)} \sup_{\mathbf{x}' \in \mathbb{R}^2} \left\| e^{c\sqrt{\lambda}\langle \cdot, -\mathbf{x}' \rangle} (H + \lambda)^{-1} (\cdot; \mathbf{x}') \right\|_{L^2(\mathbb{R}^2)} \\ & \leq C. \end{aligned} \quad (\text{A.1.40})$$

Therefore we have obtained the exponential L^∞ estimate for the second power of the resolvent, that is

$$\left| (H + \lambda)^{-2} (\mathbf{x}; \mathbf{x}') \right| \leq C e^{-c\sqrt{\lambda}\|\mathbf{x}-\mathbf{x}'\|}. \quad (\text{A.1.41})$$

Let us study how estimate (A.1.41) propagates in the resolvent set. The strategy is the same as before. In fact, consider $z \in D_\eta$, from the resolvent identity we have

$$(H - z)^{-1} = (H + \lambda)^{-1} + (z - \lambda)(H + \lambda)^{-1}(H - z)^{-1}.$$

From (A.1.39) for every $\varphi \in L^2(\mathbb{R}^2)$ we get

$$\begin{aligned} & \sup_{\mathbf{x}_0 \in \mathbb{R}^2} \sup_{\mathbf{x} \in \mathbb{R}^2} \left| \int_{\mathbb{R}^2} d\tilde{\mathbf{x}} e^{-\frac{\delta}{r}\langle \mathbf{x} - \mathbf{x}_0 \rangle} (H + \lambda)^{-1}(\mathbf{x}; \tilde{\mathbf{x}}) e^{\frac{\delta}{r}\langle \tilde{\mathbf{x}} - \mathbf{x}_0 \rangle} \varphi(\tilde{\mathbf{x}}) \right| \\ & \leq \sup_{\mathbf{x}_0 \in \mathbb{R}^2} \sup_{\mathbf{x} \in \mathbb{R}^2} \int_{\mathbb{R}^2} d\tilde{\mathbf{x}} \left| (H + \lambda)^{-1}(\mathbf{x}; \tilde{\mathbf{x}}) \right| e^{c\sqrt{\lambda}\langle \tilde{\mathbf{x}} - \mathbf{x} \rangle} \varphi(\tilde{\mathbf{x}}) \\ & \leq \sup_{\mathbf{x}_0 \in \mathbb{R}^2} \sup_{\mathbf{x} \in \mathbb{R}^2} \left\| (H + \lambda)^{-1}(\mathbf{x}; \cdot) e^{c\sqrt{\lambda}\langle \cdot - \mathbf{x} \rangle} \right\|_{L^2(\mathbb{R}^2)} \|\varphi\|_{L^2(\mathbb{R}^2)}. \end{aligned}$$

Hence

$$\sup_{\mathbf{x}_0 \in \mathbb{R}^2} \left\| e^{-\frac{\delta}{r}\langle \cdot - \mathbf{x}_0 \rangle} (H + \lambda)^{-1} e^{\frac{\delta}{r}\langle \cdot - \mathbf{x}_0 \rangle} \right\|_{\mathcal{B}(L^2, L^\infty)} \leq C.$$

This, together with the L^2 bound (A.1.32) and the resolvent identities, implies that

$$\begin{aligned} & \sup_{\mathbf{x}_0 \in \mathbb{R}^2} \left\| e^{-\frac{\delta}{r}\langle \cdot - \mathbf{x}_0 \rangle} (H - z)^{-1} e^{\frac{\delta}{r}\langle \cdot - \mathbf{x}_0 \rangle} \right\|_{\mathcal{B}(L^2, L^\infty)} \\ & \leq \sup_{\mathbf{x}_0 \in \mathbb{R}^2} \left\| e^{-\frac{\delta}{r}\langle \cdot - \mathbf{x}_0 \rangle} (H + \lambda)^{-1} e^{\frac{\delta}{r}\langle \cdot - \mathbf{x}_0 \rangle} \right\|_{\mathcal{B}(L^2, L^\infty)} \\ & \quad + (|z| + |\lambda|) \sup_{\mathbf{x}_0 \in \mathbb{R}^2} \left\| e^{-\frac{\delta}{r}\langle \cdot - \mathbf{x}_0 \rangle} (H + \lambda)^{-1} e^{\frac{\delta}{r}\langle \cdot - \mathbf{x}_0 \rangle} \right\|_{\mathcal{B}(L^2, L^\infty)} \quad (\text{A.1.42}) \\ & \quad \cdot \sup_{\mathbf{x}_0 \in \mathbb{R}^2} \left\| e^{-\frac{\delta}{r}\langle \cdot - \mathbf{x}_0 \rangle} (H - z)^{-1} e^{\frac{\delta}{r}\langle \cdot - \mathbf{x}_0 \rangle} \right\|_{\mathcal{B}(L^2, L^2)} \\ & \leq C \frac{r}{\eta}. \end{aligned}$$

Therefore, for every function $\varphi \in C_0^\infty(\mathbb{R}^2)$, we can consider the linear functional

$$\int_{\mathbb{R}^2} d\mathbf{y} (H - z)^{-1}(\mathbf{x}_0, \mathbf{y}) e^{\frac{\delta}{r}\langle \mathbf{y} - \mathbf{x}_0 \rangle} \varphi(\mathbf{y}) \quad (\text{A.1.43})$$

which, considering the estimate in equation (A.1.16), defines a bounded linear functional and can be extended to the whole Hilbert space, then via the Riesz representation theorem we obtain that

$$\begin{aligned} & \sup_{\mathbf{x}_0 \in \mathbb{R}^2} \left\| (H - z)^{-1}(\mathbf{x}_0; \cdot) e^{\frac{\delta}{r}\langle \cdot - \mathbf{x}_0 \rangle} \right\|_{L^2(\mathbb{R}^2)} \\ & = \sup_{\mathbf{x}_0 \in \mathbb{R}^2} \left\| (H - \bar{z})^{-1}(\cdot; \mathbf{x}_0) e^{\frac{\delta}{r}\langle \cdot - \mathbf{x}_0 \rangle} \right\|_{L^2(\mathbb{R}^2)} \leq C \frac{r}{\eta}. \end{aligned} \quad (\text{A.1.44})$$

Hence we have

$$\begin{aligned}
& \sup_{\mathbf{x}, \mathbf{x}' \in \mathbb{R}^2} \left| e^{\frac{\delta}{r} \|\mathbf{x} - \mathbf{x}'\|} (H - z)^{-2}(\mathbf{x}; \mathbf{x}') \right| \\
& \leq \sup_{\mathbf{x}, \mathbf{x}' \in \mathbb{R}^2} \int_{\mathbb{R}^2} d\tilde{\mathbf{x}} e^{\frac{\delta}{r} \langle \tilde{\mathbf{x}} - \mathbf{x} \rangle} \left| (H - z)^{-1}(\mathbf{x}; \tilde{\mathbf{x}}) \right| \left| (H - z)^{-1}(\tilde{\mathbf{x}}, \mathbf{x}') \right| e^{\frac{\delta}{r} \langle \tilde{\mathbf{x}} - \mathbf{x}' \rangle} \\
& \leq \sup_{\mathbf{x} \in \mathbb{R}^2} \left\| (H - z)^{-1}(\mathbf{x}; \cdot) e^{\frac{\delta}{r} \langle \cdot - \mathbf{x} \rangle} \right\|_{L^2(\mathbb{R}^2)} \sup_{\mathbf{x}' \in \mathbb{R}^2} \left\| e^{\frac{\delta}{r} \langle \cdot - \mathbf{x}' \rangle} (H - z)^{-1}(\cdot; \mathbf{x}') \right\|_{L^2(\mathbb{R}^2)} \\
& \leq C \frac{r^2}{\eta^2}.
\end{aligned} \tag{A.1.45}$$

Consider now the spectral projection P_μ . Using the Riesz formula together with integration by parts we get

$$P_\mu = -\frac{i}{2\pi} \oint_{\mathcal{C}} z (H - z)^{-2}, \tag{A.1.46}$$

which together with (A.1.45) implies that

$$\sup_{\mathbf{x}, \mathbf{x}' \in \mathbb{R}^2} \left| e^{\frac{\delta}{r} \|\mathbf{x} - \mathbf{x}'\|} P_\mu(\mathbf{x}; \mathbf{x}') \right| \leq C. \tag{A.1.47}$$

It remains to show that the kernel is jointly continuous. We use the strategy delineated above for the integral kernel of the powers of the resolvent.

Consider the trivial identity

$$g_U P_\mu g_U = (H - z)^{-1} (H - z) g_U P_\mu g_U (H - z) (H - z)^{-1}.$$

We first prove that $(H - z) g_U P_\mu g_U (H - z)$ is a Hilbert–Schmidt operator. Indeed by commuting the resolvents with the g_U we obtain

$$\begin{aligned}
& g_U P_\mu (H - z)^2 g_U \\
& + g_U P_\mu (H - z)^2 \left((H - z)^{-1} 2i \sum_{i=1}^2 (\mathbf{P}_A)_i \partial_i g_U - (H - z)^{-1} \Delta(g_U) \right) \\
& + \left(-2i \sum_{i=1}^2 \partial_i g_U (\mathbf{P}_A)_i (H - z)^{-1} + \Delta(g_U) (H - z)^{-1} \right) (H - z)^2 P_\mu g_U \\
& + \left(-2i \sum_{i=1}^2 \partial_i g_U (\mathbf{P}_A)_i (H - z)^{-1} + \Delta(g_U) (H - z)^{-1} \right) P_\mu (H - z)^2 \\
& \cdot \left((H - z)^{-1} 2i \sum_{i=1}^2 (\mathbf{P}_A)_i \partial_i g_U - (H - z)^{-1} \Delta(g_U) \right).
\end{aligned} \tag{A.1.48}$$

From (A.1.47) we have that $g_U P_\mu$ and $P_\mu g_U$ are Hilbert–Schmidt operators, indeed

$$\left| g_U e^{\|\cdot\|} \cdot \| e^{-\|\cdot\|} P_\mu(\mathbf{x}; \mathbf{x}') \right| \leq C e^{-\|\mathbf{x}\|} e^{-\frac{\delta}{r} \|\mathbf{x} - \mathbf{x}'\|},$$

hence the kernel is $L^2(\mathbb{R}^2 \times \mathbb{R}^2)$. A similar argument, together with (A.1.29) and the boundedness of $P_\mu (H - z)^2$ shows that the first three terms of (A.1.48) are Hilbert–Schmidt operators. From (A.1.33) and by commuting $(\mathbf{P}_A)_i$ with the exponential weight, it is not difficult to deduce that

$$\left\| e^{\pm \frac{\delta}{r} \langle \cdot - \mathbf{x}_0 \rangle} (\mathbf{P}_A)_i (H - z)^{-1} e^{\mp \frac{\delta}{r} \langle \cdot - \mathbf{x}_0 \rangle} \right\| \leq C.$$

Therefore one can show that also the last term is Hilbert–Schmidt, because the operator $e^{-\frac{\delta}{r}\langle \cdot - \mathbf{x}_0 \rangle} P_\mu$ is Hilbert–Schmidt and

$$\begin{aligned} & -2i \sum_{i=1}^2 \partial_i g_U e^{\frac{\delta}{r}\langle \cdot - \mathbf{x}_0 \rangle} e^{-\frac{\delta}{r}\langle \cdot - \mathbf{x}_0 \rangle} (\mathbf{P}_A)_i (H - z)^{-1} e^{\frac{\delta}{r}\langle \cdot - \mathbf{x}_0 \rangle}, \\ & \Delta(g_U) e^{\frac{\delta}{r}\langle \cdot - \mathbf{x}_0 \rangle} e^{-\frac{\delta}{r}\langle \cdot - \mathbf{x}_0 \rangle} (H - z)^{-1} e^{\frac{\delta}{r}\langle \cdot - \mathbf{x}_0 \rangle}, \end{aligned}$$

are bounded operators. Therefore, the operator $(H - z) g_U (H - z)^{-N} g_U (H - z)$ admits an integral kernel, call it $W(\mathbf{x}; \mathbf{x}')$, and hence W has to be in $L^2(\mathbb{R}^2 \times \mathbb{R}^2)$. By definition of tensor product of Hilbert space, W can be approximated in the $L^2(\mathbb{R}^2 \times \mathbb{R}^2)$ norm by a finite sum of the form

$$\sum_{j=1}^N g_j(\mathbf{x}) f_j(\mathbf{x}'),$$

with $g_j, f_j \in L^2(\mathbb{R}^2)$. By mimicking the proof of the joint continuity of $(H - z)^{-N}$ one can conclude that the integral kernel of P_μ is jointly continuous for every $\mathbf{x}, \mathbf{x}' \in \mathbb{R}^2$.

A.2 “Black boxes” of Chapter 5

In this section we will provide more details and appropriate references for a number of tools and “black boxes” employed in Chapter 5. This section reproduces the content of the Appendix of [33].

A.2.1 Smoothing argument

We start by providing a smoothing argument that allows to produce *real-analytic* Bloch vectors from continuous ones.

Lemma A.2.1 (Smoothing argument). *Let $\{P(\mathbf{k})\}_{\mathbf{k} \in \mathbb{R}^d}$ be a family of orthogonal projections admitting an analytic, \mathbb{Z}^d -periodic analytic extension to a complex strip around $\mathbb{R}^d \subset \mathbb{C}^d$. Assume that there exist continuous, \mathbb{Z}^d -periodic, and orthogonal Bloch vectors $\{\xi_1, \dots, \xi_m\}$ for $\{P(\mathbf{k})\}_{\mathbf{k} \in \mathbb{R}^d}$. Then, there exist also real-analytic, \mathbb{Z}^d -periodic, and orthogonal Bloch vectors $\{\widehat{\xi}_1, \dots, \widehat{\xi}_m\}$.*

The same holds true if analyticity is replaced by C^r -smoothness for some $r \in \mathbb{N} \cup \{\infty\}$.

Proof (sketch). We sketch here the proof: more details can be found in [30, Sec. 2.3].

Define

$$g(\mathbf{k}) = g(k_1, \dots, k_d) := \frac{1}{\pi^d} \prod_{j=1}^d \frac{1}{1 + k_j^2}.$$

The function g is analytic over the strip

$$\left\{ \mathbf{z} = (z_1, \dots, z_d) \in \mathbb{C}^d : |\operatorname{Im} z_j| < 1, j \in \{1, \dots, d\} \right\}$$

and obeys $\int_{\mathbb{R}^d} g(\mathbf{k}) d\mathbf{k} = 1$. For $\delta > 0$, define $g_\delta(\mathbf{k}) := \delta^{-d}g(\mathbf{k}/\delta)$. Set

$$\psi_a^{(\delta)}(\mathbf{k}) := \int_{\mathbb{R}^d} g_\delta(\mathbf{k} - \mathbf{k}') \xi_a(\mathbf{k}') d\mathbf{k}', \quad a \in \{1, \dots, m\}, \mathbf{k} \in \mathbb{R}^d.$$

The above define \mathbb{Z}^d -periodic vectors which admit an analytic extension to a strip of half-width δ around the real axis in \mathbb{C}^d , and moreover converge to ξ_a uniformly as $\delta \rightarrow 0$. We note here that an alternative way of smoothing has been suggested to us by G. Panati: he proposed taking the convolution with the Fejér kernel, which has the advantage of integrating on $[-1/2, 1/2]^d$ and not on the whole \mathbb{R}^d .

Now denote $\phi_a^{(\delta)}(\mathbf{k}) := P(\mathbf{k}) \psi_a^{(\delta)}(\mathbf{k})$, for $a \in \{1, \dots, m\}$ and $\mathbf{k} \in \mathbb{R}^d$. Then for any $\epsilon > 0$ there exists $\delta > 0$ such that $\phi_a^{(\delta)}(\mathbf{k})$ and $\xi_a(\mathbf{k})$ are uniformly at a distance less than ϵ . Moreover, as the ξ_a 's are orthogonal, we can make sure that the Gram-Schmidt matrix $S^{(\delta)}(\mathbf{k})_{ab} := \langle \phi_a^{(\delta)}(\mathbf{k}), \phi_b^{(\delta)}(\mathbf{k}) \rangle$ is close to the identity matrix, uniformly in \mathbf{k} , possibly at the price of choosing an even smaller δ . This implies that $S^{(\delta)}(\mathbf{k})^{-1/2}$ is real-analytic and \mathbb{Z}^d -periodic, and hence the vectors

$$\widehat{\xi}_a(\mathbf{k}) := \sum_{b=1}^m \phi_b^{(\delta)}(\mathbf{k}) \left[S^{(\delta)}(\mathbf{k})^{-1/2} \right]_{ba}$$

define the required real-analytic, \mathbb{Z}^d -periodic, and orthogonal Bloch vectors. \square

A.2.2 Parallel transport

We recall here the definition of *parallel transport* associated to a smooth and \mathbb{Z}^d -periodic family of projections $\{P(k_1, \dots, k_d)\}_{(k_1, \dots, k_d) \in \mathbb{R}^d}$ acting on an Hilbert space \mathcal{H} .

Fix $i \in \{1, \dots, d\}$. For $(k_1, \dots, k_d) \in \mathbb{R}^d$, denote by $\mathbf{k} \in \mathbb{R}^D$, $D = d - 1$, the collection of coordinates different from the i -th. We use the shorthand notation $(k_1, \dots, k_d) \equiv (k_i, \mathbf{k})$ throughout this Subsection.

Define

$$A_{\mathbf{k}}(k_i) := i [\partial_{k_i} P(k_i, \mathbf{k}), P(k_i, \mathbf{k})], \quad (k_i, \mathbf{k}) \in \mathbb{R}^d. \quad (\text{A.2.1})$$

Then $A_{\mathbf{k}}(k_i)$ defines a self-adjoint operator on \mathcal{H} . The solution to the operator-valued Cauchy problem

$$i \partial_{k_i} T_{\mathbf{k}}(k_i, k_i^0) = A_{\mathbf{k}}(k_i) T_{\mathbf{k}}(k_i, k_i^0), \quad T_{\mathbf{k}}(k_i^0, k_i^0) = \mathbf{1}, \quad (\text{A.2.2})$$

defines a family of unitary operators on \mathcal{H} , called the *parallel transport unitaries* (along the i -th direction). In the following we will fix $k_i^0 = 0$. This notion coincides with the one in differential geometry of the parallel transport along the straight line from $(0, \mathbf{k})$ to (k_i, \mathbf{k}) associated to the *Berry connection* on the Bloch bundle. The parallel transport unitaries satisfy the properties listed in the following result.

Lemma A.2.2. *Let $\{P(\mathbf{k})\}_{\mathbf{k} \in \mathbb{R}^d}$ be a smooth (respectively analytic) and \mathbb{Z}^d -periodic family of orthogonal projections acting on an Hilbert space \mathcal{H} . Then the family of parallel transport unitaries $\{T_{\mathbf{k}}(k_i, 0)\}_{k_i \in \mathbb{R}, \mathbf{k} \in \mathbb{R}^D}$ defined in (A.2.2) satisfies the following properties:*

(i) the map $\mathbb{R}^d \ni \mathbf{k} = (k_i, \mathbf{k}) \mapsto T_{\mathbf{k}}(k_i, 0) \in \mathcal{U}(\mathcal{H})$ is smooth (respectively real-analytic);

(ii) for all $k_i \in \mathbb{R}$ and $\mathbf{k} \in \mathbb{R}^D$

$$T_{\mathbf{k}}(k_i + 1, 1) = T_{\mathbf{k}}(k_i, 0)$$

and

$$T_{\mathbf{k}+\mathbf{n}}(k_i, 0) = T_{\mathbf{k}}(k_i, 0) \quad \text{for } \mathbf{n} \in \mathbb{Z}^D;$$

(iii) the intertwining property

$$P(k_i, \mathbf{k}) = T_{\mathbf{k}}(k_i, 0) P(0, \mathbf{k}) T_{\mathbf{k}}(k_i, 0)^{-1}$$

holds for all $k_i \in \mathbb{R}$ and $\mathbf{k} \in \mathbb{R}^D$.

A proof of all these properties can be found for example in [49] or in [30, Sec. 2.6].

In (5.5.2), the parallel transport unitary $\mathcal{T}(\mathbf{k}) := T_{\mathbf{k}}(1, 0)$ is employed to define the continuous, \mathbb{Z}^D -periodic family of unitary matrices $\{\alpha(\mathbf{k})\}_{\mathbf{k} \in \mathbb{R}^D}$. Let $j \in \{1, \dots, d\}$, $j \neq i$. The integrand in the formula (5.5.3) for $\deg_j(\det \alpha)$ can be expressed in terms of the parallel transport unitaries as

$$\mathrm{tr}_{\mathbb{C}^m} \left(\alpha(\mathbf{k})^* \partial_{k_j} \alpha(\mathbf{k}) \right) = \mathrm{Tr}_{\mathcal{H}} \left(P(0, \mathbf{k}) \mathcal{T}(\mathbf{k})^* \partial_{k_j} \mathcal{T}(\mathbf{k}) \right)$$

(compare [34, Lemma 6.1]). Besides, by the Duhamel formula we have

$$\partial_{k_j} T_{\mathbf{k}}(k_i, 0) = T_{\mathbf{k}}(k_i, 0) \int_0^{k_i} ds T_{\mathbf{k}}(s, 0)^* \partial_{k_j} A_{\mathbf{k}}(s) T_{\mathbf{k}}(s, 0),$$

where $A_{\mathbf{k}}(s)$ is as in (A.2.1) (compare [34, Lemma 6.2]). On the other hand, one can also compute

$$P(k_i, \mathbf{k}) \partial_{k_j} A_{\mathbf{k}}(k_i) P(k_i, \mathbf{k}) = P(k_i, \mathbf{k}) [\partial_{k_i} P(k_i, \mathbf{k}), \partial_{k_j} P(k_i, \mathbf{k})] P(k_i, \mathbf{k})$$

so that, denoting $\mathbf{K} := (k_i, \mathbf{k}) \in \mathbb{R}^d$,

$$\mathrm{Tr}_{\mathcal{H}} \left(P(0, \mathbf{k}) \mathcal{T}(\mathbf{k})^* \partial_{k_j} \mathcal{T}(\mathbf{k}) \right) = \int_0^1 dk_i \mathrm{Tr}_{\mathcal{H}} \left(P(\mathbf{K}) \left[\partial_{k_i} P(\mathbf{K}), \partial_{k_j} P(\mathbf{K}) \right] \right)$$

(compare [34, Eqn. (6.13)]). Putting all the above equalities together, we conclude that

$$\deg_j(\det \alpha) = \frac{1}{2\pi i} \int_0^1 dk_j \int_0^1 dk_i \mathrm{Tr}_{\mathcal{H}} \left(P(\mathbf{K}) \left[\partial_{k_i} P(\mathbf{K}), \partial_{k_j} P(\mathbf{K}) \right] \right) = c_1(P)_{ij},$$

see (5.3.2). The above equality proves Proposition 5.5.3 as well as Equation (5.5.8).

A.2.3 Cayley transform

An essential tool to produce “good” logarithms for families of unitary matrices which inherit properties like continuity and (γ) -periodicity is the *Cayley transform*. We recall here this construction.

Lemma A.2.3 (Cayley transform). *Let $\{\alpha(\mathbf{k})\}_{\mathbf{k} \in \mathbb{R}^D}$ be a family of unitary matrices which is continuous and \mathbb{Z}^D -periodic. Assume that -1 lies in the resolvent set of $\alpha(\mathbf{k})$ for all $\mathbf{k} \in \mathbb{R}^D$. Then one can construct a family $\{h(\mathbf{k})\}_{\mathbf{k} \in \mathbb{R}^D}$ of self-adjoint matrices which is continuous, \mathbb{Z}^D -periodic and such that*

$$\alpha(\mathbf{k}) = e^{i h(\mathbf{k})} \quad \text{for all } \mathbf{k} \in \mathbb{R}^D.$$

If $D = 2$ and $\{\alpha(k_2, k_3)\}_{(k_2, k_3) \in \mathbb{R}^2}$ is γ -periodic (in the sense of Definition 5.6.1), then the above family of self-adjoint matrices can be chosen to be γ -periodic as well.

Proof. The proof adapts the one in [34, Prop. 3.5]. The Cayley transform

$$s(\mathbf{k}) := i (\mathbf{1} - \alpha(\mathbf{k})) (\mathbf{1} + \alpha(\mathbf{k}))^{-1}$$

is self-adjoint, depends continuously on \mathbf{k} , and is \mathbb{Z}^D -periodic (respectively γ -periodic) if α is as well. One also immediately verifies that

$$\alpha(\mathbf{k}) = (\mathbf{1} + i s(\mathbf{k})) (\mathbf{1} - i s(\mathbf{k}))^{-1}.$$

Let \mathcal{C} be a closed, positively-oriented contour in the complex plane which encircles the real spectrum of $s(\mathbf{k})$ for all $\mathbf{k} \in \mathbb{R}^D$. Let $\log(\cdot)$ denote the choice of the complex logarithm corresponding to the branch cut on the negative real semi-axis. Then

$$h(\mathbf{k}) := \frac{1}{2\pi} \oint_{\mathcal{C}} \log \left(\frac{1 + iz}{1 - iz} \right) (s(\mathbf{k}) - z\mathbf{1})^{-1} dz, \quad \mathbf{k} \in \mathbb{R}^D,$$

obeys all the required properties. □

A.2.4 Generically non-degenerate spectrum of families of unitary matrices

The aim of this Subsection is to prove that

Proposition A.2.4. *Let $D \leq 2$. Consider a continuous and \mathbb{Z}^D -periodic family of unitary matrices $\{\alpha(\mathbf{k})\}_{\mathbf{k} \in \mathbb{R}^D}$. Then, one can construct a sequence of continuous, \mathbb{Z}^D -periodic families of unitary matrices $\{\alpha_n(\mathbf{k})\}_{\mathbf{k} \in \mathbb{R}^D}$, $n \in \mathbb{N}$, such that*

- $\sup_{\mathbf{k} \in \mathbb{R}^D} \|\alpha_n(\mathbf{k}) - \alpha(\mathbf{k})\| \rightarrow 0$ as $n \rightarrow \infty$, and
- the spectrum of $\alpha_n(\mathbf{k})$ is completely non-degenerate for all $n \in \mathbb{N}$ and $\mathbf{k} \in \mathbb{R}^D$.

In $D = 2$, the same conclusion holds if periodicity and homotopy are replaced by γ -periodicity and γ -homotopy, in the sense of Definition 5.6.1.

The periodic case for $D \leq 2$ has already been treated in [30], [34] and [31], but we will sketch below the main ideas and give details on the new, γ -periodic situation.

We will need two technical results, which we state here.

Lemma A.2.5 (Analytic Approximation Lemma). *Consider a uniformly continuous family of unitary matrices $\alpha(k)$ where $k \in [a, b] \subset \mathbb{R}$. Let I be any compact set completely included in $[a, b]$. Then one can construct a sequence $\{\alpha_n(k)\}_{k \in I}$, $n \in \mathbb{N}$, of families of unitary matrices which are real-analytic on I and such that*

$$\sup_{k \in I} \|\alpha_n(k) - \alpha(k)\| \rightarrow 0 \quad \text{as } n \rightarrow \infty.$$

If α is continuous and \mathbb{Z} -periodic, the same is true for α_n and the approximation is uniform on \mathbb{R} . This last statement can be extended to any $D \geq 1$.

Proof (sketch). The proof proceeds in the same spirit of Lemma A.2.1 above. First, we take the convolution with a real-analytic kernel and obtain a smooth matrix $\beta(k)$ which is close in norm to $\alpha(k)$. Thus $\kappa := \beta^* \beta$ must be close to the identity matrix, it is self-adjoint and real-analytic, and the same holds true for $\kappa^{1/2}$. Finally, we restore unitarity by writing $\alpha' := \beta \kappa^{1/2}$ and checking that $(\alpha')^* \alpha' = \mathbf{1}$. More details can be found in [34, Lemma A.2]. \square

Lemma A.2.6 (Local Splitting Lemma). *For $R > 0$ and $\mathbf{k}_0 \in \mathbb{R}^D$, denote by $B_R(\mathbf{k}_0)$ the open ball of radius R around \mathbf{k}_0 . Let $\{\alpha(\mathbf{k})\}_{\mathbf{k} \in B_R(\mathbf{k}_0)}$ be a continuous family of unitary matrices. Then, for some $R' \leq R$, one can construct a sequence $\{\alpha_n(\mathbf{k})\}_{\mathbf{k} \in B_{R'}(\mathbf{k}_0)}$, $n \in \mathbb{N}$, of continuous families of unitary matrices such that*

- $\sup_{\mathbf{k} \in B_{R'}(\mathbf{k}_0)} \|\alpha_n(\mathbf{k}) - \alpha(\mathbf{k})\| \rightarrow 0$ as $n \rightarrow \infty$, and
- the spectrum of $\alpha_n(\mathbf{k})$ is completely non-degenerate for all $\mathbf{k} \in B_{R'}(\mathbf{k}_0)$.

The proof of the above lemma can be found in [34, Lemma A.1] for $D = 1$ and in [31, Lemma 5.1] for $D = 2$.

Proof of Proposition A.2.4. The main idea is to lift all the spectral degeneracies of α within the unit interval $[0, 1]$ or the unit square $[0, 1] \times [0, 1]$, and then extend the approximants with non-degenerate spectrum to the whole \mathbb{R}^D by either periodicity or γ -periodicity.

We start with $D = 1$. By the Analytic Approximation Lemma we can find an approximant $\alpha^{(1)}$ of α which depends analytically on k . If $\alpha^{(1)}$ has degenerate eigenvalues, then they either cross at isolated points (a finite number of them in the compact interval $[0, 1]$) or they stay degenerate for all $k \in [0, 1]$. Pick a point in $[0, 1]$ which is not an isolated degenerate point. Applying the Local Splitting Lemma, find a continuous approximant $\alpha^{(2)}$ of $\alpha^{(1)}$ for which the second option is ruled out, so that its eigenvalues cannot be constantly degenerate.

Let now $\alpha^{(3)}$ be an analytic approximation of $\alpha^{(2)}$, obtained by means of the Analytic Approximation Lemma. The eigenvalues of $\alpha^{(3)}$ can only be degenerate at a finite number of points $\{0 < k_1 < \dots < k_S < 1\}$ (we assume without loss of generality that no eigenvalue intersections occur at $k = 0$: this can be achieved by means of small shift of the coordinate). By applying the Local Splitting Lemma to balls of radius $1/n$ around each such point (starting from a large enough n_0), and extending the definition of the approximants from $[0, 1]$ to \mathbb{R} by periodicity, we obtain the required continuous and periodic approximants α_n with completely

non-degenerate spectrum. Notice that, under the assumption of null-homotopy of α , the rest of the argument of Theorem 5.5.2 applies: in particular, for n sufficiently large α_n admits a continuous and periodic logarithm, namely $\alpha_n(k) = e^{i h_n(k)}$.

Now we continue with $D = 2$. We will only treat the γ -periodic setting, since the periodic case for $D \leq 2$ has been already analyzed in [30], [34] and [31].

We start by considering the strip $[0, 1] \times \mathbb{R}$. The matrix $\alpha(0, k_3)$ is periodic, hence we may find a smooth approximation $\alpha_0(k_3)$ which is always non-degenerate and periodic.

The matrix $\alpha(k_2, k_3)\alpha(0, k_3)^{-1}$ is close to the identity near $k_2 = 0$, and so is $\alpha(k_2, k_3)\alpha_0(k_3)^{-1}$. Hence if k_2 is close to 0 we can write (using the Cayley transform)

$$\alpha(k_2, k_3) = e^{iH_0(k_2, k_3)}\alpha_0(k_3)$$

where $H_0(k_2, k_3)$ is continuous, periodic in k_3 , and uniformly close to zero. Due to the γ -periodicity of α , we have that $\alpha(1, k_3)$ and $\gamma(k_3)\alpha_0(k_3)\gamma(k_3)^{-1}$ are also close in norm. Reasoning in the same way as near $k_2 = 0$ we can write

$$\alpha(k_2, k_3) = e^{iH_1(k_2, k_3)}\gamma(k_3)\alpha_0(k_3)\gamma(k_3)^{-1}$$

where $H_1(k_2, k_3)$ is continuous, periodic in k_3 , and uniformly close to zero near $k_2 = 1$.

Let $\delta < 1/10$. Choose a smooth function $0 \leq g_\delta \leq 1$ such that

$$g_\delta(k_2) = \begin{cases} 1 & \text{if } k_2 \in [0, \delta] \cup [1 - \delta, 1], \\ 0 & \text{if } 2\delta \leq k_2 \leq 1 - 2\delta. \end{cases}$$

For $0 \leq k_2 \leq 1$ and $k_3 \in \mathbb{R}$, define the matrix $\alpha_\delta(k_2, k_3)$ in the following way:

$$\alpha_\delta(k_2, k_3) := \begin{cases} e^{i(1-g_\delta(k_2))H_0(k_2, k_3)}\alpha_0(k_3) & \text{if } 0 \leq k_2 \leq 3\delta, \\ \alpha(k_2, k_3) & \text{if } 3\delta < k_2 < 1 - 3\delta, \\ e^{i(1-g_\delta(k_2))H_1(k_2, k_3)}\gamma(k_3)\alpha_0(k_3)\gamma(k_3)^{-1} & \text{if } 1 - 3\delta \leq k_2 \leq 1. \end{cases}$$

We notice that α_δ is continuous, periodic in k_3 and converges in norm to α when δ goes to zero. Moreover,

$$\alpha_\delta(1, k_3) = \gamma(k_3)\alpha_\delta(0, k_3)\gamma(k_3)^{-1},$$

which is a crucial ingredient if we want to continuously extend it by γ -periodicity to \mathbb{R}^2 .

We also note that $\alpha_\delta(k_2, k_3)$ is completely non-degenerate when k_2 is either 0 or 1, hence by continuity it must remain completely non-degenerate when $k_2 \in [0, \epsilon] \cup [1 - \epsilon, 1]$ if ϵ is small enough.

Following [31], we will explain how to produce an approximation $\alpha'(k_2, k_3)$ of $\alpha_\delta(k_2, k_3)$ with the following properties:

- it coincides with $\alpha_\delta(k_2, k_3)$ if $k_2 \in [0, \epsilon] \cup [1 - \epsilon, 1]$,
- it is continuous on $[0, 1] \times \mathbb{R}$ and periodic in k_3 ,

- it is completely non-degenerate on the strip $[0, 1] \times \mathbb{R}$.

Assuming for now that all this holds true, let us investigate the consequences. Because it coincides with α_δ near $k_2 = 0$ and $k_2 = 1$, we also have:

$$\alpha'(1, k_3) = \gamma(k_3)\alpha'(0, k_3)\gamma(k_3)^{-1}.$$

If $k_2 > 0$ we define recursively

$$\alpha'(k_2 + 1, k_3) = \gamma(k_3)\alpha'(k_2, k_3)\gamma(k_3)^{-1}$$

and if $k_2 < 0$

$$\alpha'(k_2, k_3) = \gamma(k_3)^{-1}\alpha'(k_2 + 1, k_3)\gamma(k_3).$$

Then α' has all the properties required in the statement, and the proof is complete.

Finally let us sketch the main ideas borrowed from [31] which are behind the proof of the three properties of α' listed above.

First, the construction of α' is based on continuously patching non-degenerate local logarithms, which is why the already non-degenerate region $k_2 \in [0, \epsilon] \cup [1 - \epsilon, 1]$ is left unchanged.

Second, let us consider the finite segment defined by $k_2 \in [\epsilon, 1 - \epsilon]$ and $k_3 = 0$. The family of matrices $\{\alpha_\delta(k_2, 0)\}$ is 1-dimensional, with a spectrum which is completely non-degenerate near $k_2 = \epsilon$ and $k_2 = 1 - \epsilon$. Reasoning as in the case $D = 1$ we can find a continuous approximation $\alpha_2(k_2)$ which is completely non-degenerate on the whole interval $k_2 \in [\epsilon, 1 - \epsilon]$. The matrix $\alpha_\delta(k_2, k_3)\alpha_2(k_2)^{-1}$ is close to the identity matrix if $|k_3| \ll 1$, hence we may locally perturb α_δ near the segment $(\epsilon, 1 - \epsilon) \times \{0\}$ so that the new α'_δ is completely non-degenerate on a small tubular neighborhood of the boundary of the segment $(\epsilon, 1 - \epsilon) \times \{0\}$. This perturbation must be taken small enough not to destroy the initial non-degeneracy near $k_2 = \epsilon$ and $k_2 = 1 - \epsilon$.

Third, since α_δ is periodic in k_3 , the local perturbation around the strip $(\epsilon, 1 - \epsilon) \times \{0\}$ can be repeated near all the strips $(\epsilon, 1 - \epsilon) \times \mathbb{Z}$. The new matrix, α''_δ , will be non-degenerate near a small tubular neighborhood of any unit square of the type $[0, 1] \times [p, p + 1]$, with $p \in \mathbb{Z}$. The final step is to locally perturb α''_δ inside these squares, like in [31, Prop. 5.11]. The splitting method relies in an essential way on the condition $D \leq 2$, since it uses the fact that a smooth map between \mathbb{R}^D and \mathbb{R}^3 cannot have regular values. \square

A.2.5 Resolvent estimates

In this final Appendix we will prove the estimates on the matrix elements of the resolvent of the Hamiltonian \mathcal{H}_ϵ that we used in Section 5.8.

Proposition A.2.7 (Combes–Thomas type estimate). *Consider an operator H_0 in $\ell^2(\mathbb{Z}^2) \otimes \mathbb{C}^Q$ such that its matrix elements are localized along the diagonal, that is,*

$$|H_0(\gamma, \underline{x}; \gamma', \underline{x}')| \leq C e^{-\beta_0 \|\gamma - \gamma'\|} \quad \forall \gamma, \gamma' \in \mathbb{Z}^2, \quad \underline{x}, \underline{x}' \in \{1, \dots, Q\}$$

for some positive constants C and β_0 . Moreover fix a compact set $K \subset \rho(\mathcal{H}_0)$. Then, there exist two constants C' and $0 < \beta < \beta_0$ such that

$$\sup_{z \in K} \left\| (H_0 - z)^{-1}(\gamma, \underline{x}; \gamma', \underline{x}') \right\| \leq C' e^{-\beta \|\gamma - \gamma'\|}, \quad \forall \gamma, \gamma' \in \mathbb{Z}^2, \quad \underline{x}, \underline{x}' \in \{1, \dots, Q\}.$$

Proof. Take $\gamma_0 \in \mathbb{Z}^2$. Consider the operator $H_\beta^{(\gamma_0)}$ defined by the following matrix elements:

$$H_\beta^{(\gamma_0)}(\gamma, \underline{x}; \gamma', \underline{x}') := e^{\beta\|\gamma-\gamma_0\|} H_0(\gamma, \underline{x}; \gamma', \underline{x}') e^{-\beta\|\gamma'-\gamma_0\|}, \quad (\text{A.2.3})$$

for all $\gamma, \gamma' \in \mathbb{Z}^2$, and $\underline{x}, \underline{x}' \in \{1, \dots, Q\}$. Using the inequality $|e^x - 1| \leq |x|e^{|x|}$, which holds for all $x \in \mathbb{R}$, together with the triangle inequality we have

$$\sup_{\gamma_0 \in \mathbb{Z}^2} \left| H_\beta^{(\gamma_0)}(\gamma, \underline{x}; \gamma', \underline{x}') - H_0(\gamma, \underline{x}; \gamma', \underline{x}') \right| \leq C\beta\|\gamma - \gamma'\| e^{-(\beta_0 - \beta)\|\gamma - \gamma'\|}. \quad (\text{A.2.4})$$

Using a Schur–Holmgren estimate, as soon as $\beta < \beta_0$ we get from (A.2.4) that $\|H_\beta^{(\gamma_0)} - H_0\| \leq \beta C$ for all γ_0 . If $z \in K \subset \rho(H_0)$, we can choose a β small enough such that the operator

$$\left(\mathbf{1} + \left(H_\beta^{(\gamma_0)} - H_0 \right) (H_0 - z)^{-1} \right)$$

is invertible uniformly in z and γ_0 . Thus we obtain that

$$(H_\beta^{(\gamma_0)} - z)^{-1} = (H_0 - z)^{-1} \left(\mathbf{1} + \left(H_\beta^{(\gamma_0)} - H_0 \right) (H_0 - z)^{-1} \right)^{-1},$$

which implies

$$\sup_{\gamma_0 \in \mathbb{Z}^2} \sup_{z \in K} \left\| \left(H_\beta^{(\gamma_0)} - z \right)^{-1} \right\| =: A < \infty. \quad (\text{A.2.5})$$

Also, β only depends on the minimal distance between z and the spectrum of H_0 .

We are now ready to prove the exponential localization of the resolvent of H_0 . From the definition (A.2.3) of $H_\beta^{(\gamma_0)}$ we obtain that $e^{-\beta\|\cdot-\gamma_0\|} H_\beta^{(\gamma_0)} = H_0 e^{-\beta\|\cdot-\gamma_0\|}$. From this identity and from (A.2.5) we get that for every $z \in K$

$$(H_0 - z)^{-1} e^{-\beta\|\cdot-\gamma_0\|} = e^{-\beta\|\cdot-\gamma_0\|} (H_\beta^{(\gamma_0)} - z)^{-1}. \quad (\text{A.2.6})$$

Hence (A.2.6) shows that $(H_0 - z)^{-1} e^{-\beta\|\cdot-\gamma_0\|}$ maps in the domain of the unbounded multiplication operator $e^{\beta\|\cdot-\gamma_0\|}$. Finally, considering the vector $\delta_{\gamma_0, \underline{x}'}$ that is equal to 1 only in $(\gamma_0, \underline{x}')$, and using the fact that in the discrete setting the ℓ^∞ norm is bounded by the ℓ^2 norm, (A.2.5) implies

$$\left| e^{\beta\|\gamma-\gamma_0\|} (H_0 - z)^{-1}(\gamma, \underline{x}; \gamma_0, \underline{x}') \right| = \left| \left((H_\beta^{(\gamma_0)} - z)^{-1} \delta_{\gamma_0, \underline{x}'} \right) (\gamma, \underline{x}) \right| \leq A$$

which concludes the proof. \square

For the next statement, recall that \mathcal{H}_ϵ was defined in (5.8.1).

Proposition A.2.8. *Fix a compact set $K \subset \rho(\mathcal{H}_0)$. Then there exist $\epsilon_0 > 0$, $\alpha < \infty$ and $C < \infty$ such that for every $0 \leq \epsilon \leq \epsilon_0$ we have that $K \subset \rho(\mathcal{H}_\epsilon)$ and:*

$$\sup_{z \in K} \left| (\mathcal{H}_\epsilon - z)^{-1}(\gamma, \underline{x}; \gamma', \underline{x}') - e^{i\epsilon\phi(\gamma, \gamma')} (\mathcal{H}_0 - z)^{-1}(\gamma, \underline{x}; \gamma', \underline{x}') \right| \leq C \epsilon e^{-\alpha\|\gamma-\gamma'\|}. \quad (\text{A.2.7})$$

Proof. By hypothesis we know that $|\mathcal{H}_0(\gamma, \underline{x}; \gamma', \underline{x}')| \leq C'e^{-\beta\|\gamma-\gamma'\|}$ and hence Proposition A.2.7 gives us that also $|(\mathcal{H}_0 - z)^{-1}(\gamma, \underline{x}; \gamma', \underline{x}')| \leq C''e^{-\beta\|\gamma-\gamma'\|}$, uniformly for every $z \in K$. Consider the operator $S_z^{(\epsilon)}$ defined by the following matrix elements:

$$S_z^{(\epsilon)}(\gamma, \underline{x}; \gamma', \underline{x}') := e^{i\epsilon\phi(\gamma, \gamma')}(\mathcal{H}_0 - z)^{-1}(\gamma, \underline{x}; \gamma', \underline{x}'),$$

for all $\gamma, \gamma' \in \mathbb{Z}^2$, and $\underline{x}, \underline{x}' \in \{1, \dots, Q\}$. Then consider the matrix of $(\mathcal{H}_\epsilon - z)S_z^{(\epsilon)}$. Exploiting the magnetic phase composition rule (5.9.8) and the fact that $e^{i\epsilon\phi(\gamma, \gamma)} = 1$ we get

$$(\mathcal{H}_\epsilon - z)S_z^{(\epsilon)} =: \mathbf{1} + T_z^{(\epsilon)}, \quad (\text{A.2.8})$$

where $T_z^{(\epsilon)}$ is the operator associated with the matrix elements

$$e^{i\epsilon\phi(\gamma, \gamma')} \sum_{\tilde{\gamma} \in \mathbb{Z}^2} \sum_{\tilde{\mathbf{x}}=1}^Q \left(e^{i\epsilon\phi(\gamma-\tilde{\gamma}, \tilde{\gamma}-\gamma')} - 1 \right) \mathcal{H}_0(\gamma, \underline{x}; \tilde{\gamma}, \tilde{\mathbf{x}})(\mathcal{H}_0 - z)^{-1}(\tilde{\gamma}, \tilde{\mathbf{x}}; \gamma', \underline{x}'), \quad (\text{A.2.9})$$

for all $\gamma, \gamma' \in \mathbb{Z}^2$, and $\underline{x}, \underline{x}' \in \{1, \dots, Q\}$. Now note that

$$\left| e^{i\epsilon\phi(\gamma-\tilde{\gamma}, \tilde{\gamma}-\gamma')} - 1 \right| \leq \frac{\epsilon}{2} \|\gamma - \tilde{\gamma}\| \|\tilde{\gamma} - \gamma'\|.$$

Considering the exponential localization of \mathcal{H}_0 and $(\mathcal{H}_0 - z)^{-1}$, a simple computation shows that, for every $\alpha < \beta$,

$$e^{\alpha\|\gamma-\gamma'\|} \left| T_z^{(\epsilon)}(\gamma, \underline{x}; \gamma', \underline{x}') \right| \leq \tilde{C}\epsilon, \quad (\text{A.2.10})$$

where \tilde{C} is some constant independent of z . Hence a Schur–Holmgren estimate now proves that $\|T_z^{(\epsilon)}\| \leq \tilde{C}\epsilon$. So, fix an ϵ_0 such that the norm of $T_z^{(\epsilon)}$ is less than 1, then for every $\epsilon \leq \epsilon_0$ we can invert the operator $\mathbf{1} + T_z^{(\epsilon)}$. Due to the selfadjointness of \mathcal{H}_ϵ we know a priori that $(\mathcal{H}_\epsilon - z)$ is invertible for every z such that $\text{Im } z \neq 0$. So, from (A.2.8) we obtain that

$$(\mathcal{H}_\epsilon - z)^{-1} = S_z^{(\epsilon)} \left(\mathbf{1} + T_z^{(\epsilon)} \right)^{-1}$$

and

$$\left\| (\mathcal{H}_\epsilon - z)^{-1} \right\| \leq \left\| S_z^{(\epsilon)} \right\| < C,$$

where C is a constant that depends only on K and does not depend on the imaginary part of z . So we can conclude that K is also in the resolvent set of \mathcal{H}_ϵ whenever $\epsilon \leq \epsilon_0$. Finally, from (A.2.8) we have that $S_z^{(\epsilon)} - (\mathcal{H}_\epsilon - z)^{-1} = (\mathcal{H}_\epsilon - z)^{-1}T_z^{(\epsilon)}$. Since K is in the resolvent set of \mathcal{H}_ϵ , using Proposition A.2.7 we infer that $(\mathcal{H}_\epsilon - z)^{-1}$ has matrix elements localized around the diagonal, hence (A.2.7) follows taking into account (A.2.10). \square

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