

ON THE STRUCTURE OF BAND EDGES OF 2D PERIODIC ELLIPTIC OPERATORS

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To the memory of Yuri Safarov, our dear friend and colleague

ABSTRACT. For a wide class of 2D periodic elliptic operators, we show that the minima and maxima of spectral band functions are attained on at most discrete set of values of the quasi-momentum.

1. INTRODUCTION

The structure of band edges of periodic Schrödinger operators is an interesting and widely open question of mathematical physics. For example, suppose that a band function $k \mapsto E(k)$ has a minimum (or maximum) k_0 . In solid state physics, the *tensor of effective masses* M_{eff} around k_0 is defined as

$$\{M_{\text{eff}}^{-1}\}_{ij} = \pm \frac{1}{\hbar^2} \left. \frac{\partial^2 E}{\partial k_i \partial k_j} \right|_{k=k_0}.$$

(see [1, Chapter 12, (12.29)] for more details). The choice of sign depends on whether the extremum is a minimum (“+”, the effective mass of an electron) or a maximum (“−”, the effective mass of a hole). This definition of M_{eff} makes sense only if the right hand side is invertible, i. e. the critical point k_0 is non-degenerate. This is always true in one dimension, see, for example, [16, Chapter 16]. It is commonly believed that, for $d \geq 2$, the spectral gap edges are non-degenerate for “generic” potentials, see, for example, [14, Conjecture 5.1]. However, there are very few rigorous results in this direction. In [9], it is shown that the lowest eigenvalue for the periodic Schrödinger operator is non-degenerate. The same holds for the two-dimensional Pauli operator, see [5]. A wide class of operators for which the lower edge of the spectrum can be extensively analysed is described in [4]. See also the review [11] on photonic crystals, where additional references are given. For periodic *magnetic* Schrödinger operators, already the lowest eigenvalue may be degenerate [18] (note, however, that this can happen only for large enough magnetic potentials, see [19]).

Much less is known about the edges of other bands. In [10], it is established that, for periodic operators of the form $-\Delta + V$ with generic V , the extrema of band functions at the edges of spectral gaps are attained on single bands, but the question of non-degeneracy of these extrema remains open. In [21], it is shown that for any N there exists a C^∞ -neighbourhood of 0 such that, for potentials V from a dense G_δ -subset of that neighbourhood, the first N band functions are Morse functions. In other words, any finite number of bands is non-degenerate for generic C^∞ -small potentials.

In the present paper, we establish the following result (Theorem 2.1): for a wide class of 2D periodic elliptic second order operators, any maximum or minimum of any band function can only be attained on a discrete set of points. This excludes the possibility of the extrema being “very degenerate”, i. e. band functions being flat along some curves. We do not need any genericity or smallness assumptions, and our result holds for all bands, not necessarily edges of the spectrum. We formulate the results for “smooth” second order elliptic operators (2.1). We

believe that, using methods from [17], the result can be extended to the same generality in which absolute continuity of the spectrum in 2D is established. The extension beyond dimension 2, however, seems significantly more challenging, as our technique relies heavily on 2D specifics.

An immediate consequence of our result is that Liouville theorems (in the sense of [13, 14]) hold for the operator (2.1) at all gap edges, see Corollary 2.2. The result can also be used in studying Green's function asymptotics near spectral gap edges: in [8, 15] it is done under the assumption that the extremum is non-degenerate and is attained at a single point, but the last requirement can be relaxed to a finite set of points ([15, Assumption A3'] and [8, Remark 3.2]).

To our surprise, the statement of the main theorem *fails for discrete periodic Schrödinger operators on \mathbb{Z}^2* , already in the case of the potential taking two different values. We explain the corresponding example in Section 7.

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2. FORMULATION OF THE RESULT

Let

$$\Gamma = \{n_1 b_1 + n_2 b_2, n_1, n_2 \in \mathbb{Z}\}$$

be a lattice in \mathbb{R}^2 , and Ω be the elementary cell of Γ identified with \mathbb{R}^2/Γ . We will use notations such as $C_{\text{per}}^1(\Omega)$, $H_{\text{per}}^1(\Omega)$ for the classes of functions satisfying periodic boundary conditions.

The periodic magnetic Schrödinger operator with metric g is defined by the formal expression

$$(2.1) \quad (Hu)(x) = (-i\nabla - A(x))^* g(x) (-i\nabla - A(x))u(x) + V(x)u(x),$$

where the electric potential $V: \mathbb{R}^2 \rightarrow \mathbb{R}$ is assumed to satisfy

$$(2.2) \quad V(x + b_j) = V(x), \quad j = 1, 2, \quad V \in L^\infty(\Omega),$$

and the magnetic potential $A: \mathbb{R}^2 \rightarrow \mathbb{R}^2$ is also Γ -periodic and

$$(2.3) \quad A \in C_{\text{per}}^1(\Omega; \mathbb{R}^2), \quad \text{div } A = 0, \quad \int_{\Omega} A(x) dx = 0.$$

Note that the last two conditions can be imposed without loss of generality by choosing a suitable gauge. The metric g is assumed to be a Γ -periodic symmetric (2×2) -matrix function satisfying

$$(2.4) \quad g \in C_{\text{per}}^2(\Omega; M_2(\mathbb{R})), \quad g(x) \geq m_g \mathbf{1} > 0, \quad \text{where } \mathbf{1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},$$

for some real constant m_g . The operator (2.1) is a self-adjoint operator on $L^2(\mathbb{R}^2)$ with the domain being the Sobolev space $H^2(\mathbb{R}^2)$. From the standard Floquet–Bloch theory (see, for example, [16, Chapter 16]), it follows that H is unitarily equivalent to the direct integral

$$(2.5) \quad \int_{\tilde{\Omega}}^{\oplus} H(k) dk,$$

where $\tilde{\Omega}$ is the elementary cell of the dual lattice

$$\Gamma' = \{m_1 b'_1 + m_2 b'_2, m_1, m_2 \in 2\pi\mathbb{Z}\}, \quad \langle b_i, b'_j \rangle = \delta_{ij},$$

and the operators $H(k)$ are m -sectorial operators in $L^2(\Omega)$ defined on the domain $H_{\text{per}}^2(\Omega)$ by

$$(2.6) \quad H(k) = (-i\nabla + \bar{k} - A)^*g(-i\nabla + k - A) + V, \quad k \in \mathbb{C}^2.$$

The operators $H(k)$ form an analytic type A operator family (in the sense of Kato, [7]) with compact resolvent. Let us denote the eigenvalues of $H(k)$, taken in the increasing order, by $\lambda_j(k)$. These eigenvalues, considered as functions of k , are called *band functions*. These functions are Γ' -periodic and piecewise real analytic on \mathbb{R}^2 . The spectrum of H

$$\sigma(H) = \bigcup_j [\lambda_j^-, \lambda_j^+]$$

is the union of *spectral bands* $[\lambda_j^-, \lambda_j^+]$ which are the ranges of $\lambda_j(\cdot)$. It is well known (under much wider assumptions than ours, see [2, 17]) that there are no degenerate bands, i. e. we always have $\lambda_j^- < \lambda_j^+$. The bands, however, can overlap. The following main result is devoted to the structure of these functions at the edges of spectral bands.

Theorem 2.1. *Let H be an operator (2.1) with the potentials and the metric satisfying (2.2), (2.3), (2.4). Suppose that λ is a minimum or maximum of a band function $\lambda_j(\cdot)$. Then the set*

$$\{k \in \mathbb{R}^2 : \lambda_j(k) = \lambda\}$$

is finite up to Γ' -periodicity.

The following Liouville theorem at the edge of the spectrum immediately follows from Theorem 2.1, see [13, Theorem 23 and Remark 6.1] or [14, Theorem 4.4].

Corollary 2.2. *Under the assumptions of Theorem 2.1, for any $\mu \in \partial(\sigma(H))$, the space of polynomially bounded solutions of the equation*

$$(-i\nabla - A(x))^*g(x)(-i\nabla - A(x))u(x) + V(x)u(x) = \mu u(x)$$

has finite dimension.

Structure of the paper. Until Section 6, we deal with the case of the *scalar metric* $g(x) = \omega^2(x)\mathbf{1}$. The proof is based on the identity from [6] showing that the values of k_1 such that $\lambda(k_1e_1 + k_2e_2) = \lambda$ are eigenvalues of a certain non-selfadjoint operator $T_1(k_2, \lambda)$ (see Proposition 3.1 below). The main observation is that the band edges correspond to *degenerate* eigenvalues of that operator. The operator T_1 is introduced in Section 3, and the main result can easily be derived from Theorem 3.3. In Section 4, we show that the condition of the operator $T_1(k_2, \lambda)$ having degenerate eigenvalues is an analytic type condition. Hence, either the set of “degenerate” k_2 is discrete, or the operator $T_1(k_2, \lambda)$ has degenerate eigenvalues for all $k_2 \in \mathbb{C}$. In Section 5, we show that the latter case is impossible for the free operator and hence, using perturbation theory and estimates on the symbol, for the perturbed operator. Section 6 describes the reduction of a general C^2 -metric to a scalar one. In Section 7, we give an example of a *discrete* periodic Schrödinger operator for which the statement of the main theorem fails.

3. THE OPERATOR $T_1(k_2, \lambda)$

In this section, we deal with the operator family

$$(3.1) \quad H(k) = (-i\nabla + \bar{k} - A)^*\omega^2(-i\nabla + k - A) + V,$$

where

$$(3.2) \quad \omega \in C_{\text{per}}^2(\Omega)$$

is a scalar function such that the metric $g(x) = \omega^2(x)\mathbf{1}$ satisfies (2.4). The family (3.1), as well as (2.6), is an analytic type A operator family in the sense of [7]. This means that the domains $\text{Dom } H(k)$ do not depend on k , and $H(k)u$ is a (weakly) analytic vector-valued function of k_1 and k_2 for any $u \in \text{Dom } H(k) = \mathbf{H}_{\text{per}}^2(\Omega)$.

Since the statement of the main result is invariant under rotations and dilations of \mathbb{R}^2 , we can fix the following choice of basis in terms of the dual lattice:

$$(3.3) \quad b'_1 = \alpha e_1, \quad b'_2 = \beta e_1 + e_2, \quad \text{where } \alpha, \beta \in \mathbb{R}.$$

We also denote the coordinates of k in the *standard* basis by k_1, k_2 , that is, $k = k_1 e_1 + k_2 e_2$, and we will often denote $H(k) = H(k_1 e_1 + k_2 e_2)$ by $H(k_1, k_2)$.

In the Hilbert space $\mathbf{H}_{\text{per}}^1(\Omega) \oplus \mathbf{L}^2(\Omega)$, consider the following unbounded nonselfadjoint operator family:

$$(3.4) \quad T_1(k_2, \lambda) := \begin{pmatrix} 0 & \omega^{-2}I \\ -(H(0, k_2) - \lambda) & 2(i\partial_1 + A_1) - 2i\omega^{-1}\partial_1\omega \end{pmatrix},$$

where $\text{Dom}(T_1(k_2, \lambda)) = \mathbf{H}_{\text{per}}^2(\Omega) \oplus \mathbf{H}_{\text{per}}^1(\Omega)$, and $\partial_i = \frac{\partial}{\partial x_i}$.

Proposition 3.1. *The operators $T_1(k_2, \lambda)$ satisfy the following properties.*

- (i) *For all $k_2, \lambda \in \mathbb{C}$, the operator $T_1(k_2, \lambda)$ is closed on the domain $\mathbf{H}_{\text{per}}^2(\Omega) \oplus \mathbf{H}_{\text{per}}^1(\Omega)$. As a consequence, the family $T_1(\cdot, \lambda)$ is an analytic type A operator family.*
- (ii) *$k_1 \in \sigma(T_1(k_2, \lambda))$ if and only if $\lambda \in \sigma(H(k))$, where $k = k_1 e_1 + k_2 e_2$.*
- (iii) *For each $k_1 \in \mathbb{C} \setminus \sigma(T(k_2, \lambda))$, the resolvent $\left(T_1(k_2, \lambda) - k_1 \begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix}\right)^{-1}$ is compact in $\mathbf{H}_{\text{per}}^1(\Omega) \oplus \mathbf{L}^2(\Omega)$.*
- (iv) *The set $\sigma(T_1(k_2, \lambda))$ is $2\pi\alpha$ -periodic.*

Proof. Part (i) is standard. To establish (iii), note that a simple computation shows that the equation

$$\left(T_1(k_2, \lambda) - k_1 \begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix}\right) \begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} f \\ g \end{pmatrix}$$

has a solution of the form

$$(3.5) \quad \begin{aligned} u &= (H(k) - \lambda)^{-1} \{(2i\partial_1 + 2A_1 - 2i\omega^{-1}\partial_1\omega - k_1)\omega^2 f - g\}, \\ v &= \omega^2(f + k_1 u), \end{aligned}$$

from which it follows that, if $R(k, \lambda) = (H(k) - \lambda)^{-1}$,

$$\begin{aligned} \left(T_1(k_2, \lambda) - k_1 \begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix}\right)^{-1} \begin{pmatrix} f \\ g \end{pmatrix} &= \begin{pmatrix} 0 & 0 \\ \omega^2 I & 0 \end{pmatrix} \begin{pmatrix} f \\ g \end{pmatrix} + \\ &+ \begin{pmatrix} I & 0 \\ 0 & k_1 \omega^2 \end{pmatrix} R(k, \lambda) \begin{pmatrix} (2i\partial_1 + 2A_1(x) - k_1 - 2i\omega^{-1}(\partial_1\omega)) & -I \\ (2i\partial_1 + 2A_1(x) - k_1 - 2i\omega^{-1}(\partial_1\omega)) & -I \end{pmatrix} \begin{pmatrix} \omega^2 & 0 \\ 0 & I \end{pmatrix} \begin{pmatrix} f \\ g \end{pmatrix}. \end{aligned}$$

The first term is essentially the embedding $\mathbf{H}_{\text{per}}^1(\Omega) \subset \mathbf{L}^2(\Omega)$, which is compact, and the second term is compact since $R(k, \lambda)$ is bounded as an operator from $\mathbf{L}^2(\Omega)$ to $\mathbf{H}_{\text{per}}^2(\Omega)$ and hence is compact from $\mathbf{L}^2(\Omega)$ to $\mathbf{H}_{\text{per}}^1(\Omega)$. The computation used to obtain (3.5), in fact, establishes that if $\begin{pmatrix} u \\ v \end{pmatrix}$ is an eigenfunction of $T_1(k_2, \lambda)$ with the eigenvalue k_1 , then $H(k)u = \lambda u$. Conversely, if

$H(k)u = \lambda u$, then $u \in H_{\text{per}}^2(\Omega)$, and

$$T_1(k_2, \lambda) \begin{pmatrix} u \\ k_1 \omega^2 u \end{pmatrix} = k_1 \begin{pmatrix} u \\ k_1 \omega^2 u \end{pmatrix}.$$

This completes the proofs of (iii) and (ii).

Part (iv) follows from the fact that $H(k)$ is unitarily equivalent to $H(k + b')$ for any $b' \in \Gamma'$, and so $H(k_1, k_2)$ is unitarily equivalent to $H(k_1 + 2\pi\alpha, k_2)$. ■

In the sequel, by “multiplicity of an isolated eigenvalue” we will mean *algebraic multiplicity*, i. e. the dimension of the range of the corresponding Riesz projection. We will call an eigenvalue *degenerate* if its algebraic multiplicity is greater than or equal to 2. Otherwise, an eigenvalue is called *simple*.

Lemma 3.2. *Suppose that a band function $\lambda_j(\cdot)$ attains its local minimum or maximum value λ_* at $k = k_1 e_1 + k_2 e_2$. Then k_1 is an eigenvalue of $T_1(k_2, \lambda_*)$ of (algebraic) multiplicity at least two.*

Proof. For some $\varepsilon > 0$, there are no other eigenvalues of $T_1(k_2, \lambda_*)$ within the closed ball $\overline{B_\varepsilon(k_1)}$. Denote by $P(k_2, \lambda)$ the Riesz projection of $T_1(k_2, \lambda)$ onto the subspace corresponding to the interior of this ball. The standard arguments show that, for some $\delta > 0$, $\text{rank } P(k_2, \lambda)$ is continuous in λ as long as $|\lambda - \lambda_*| < \delta$. Without loss of generality, assume that k is a local minimum of $\lambda_j(\cdot)$.

From the proofs of absolute continuity of the spectrum (for example, [2]), it follows that $\lambda_j(k)$ cannot be constant in k_1 . Then, for sufficiently small δ and fixed k_2 , the equation $\lambda_j(k_1, k_2) = \lambda_* + \delta$ has at least two different solutions as an equation in k_1 . Hence, $\text{rank } P(k_2, \lambda_* + \delta) \geq 2$ for all sufficiently small δ , and therefore $\text{rank } P(k_2, \lambda_*) \geq 2$ due to continuity. ■

The following is the main technical result of the paper.

Theorem 3.3. *Suppose that the coefficients ω, A, V satisfy (3.2), (2.3), (2.2). For any $\lambda \in \mathbb{R}$, the set*

$$\{k_2 \in \mathbb{R} : \text{the operator } T_1(k_2, \lambda) \text{ has at least one real degenerate eigenvalue}\}$$

is discrete.

Proof of Theorem 2.1: the case of a scalar metric. Fix $\lambda \in \mathbb{R}$ and a band function $\lambda_j(\cdot)$. From Theorem 3.3 and Lemma 3.2, the set of possible k_2 such that for some k_1 we have $\lambda_j(k) = \lambda$, is discrete. For each of these k_2 , the set of possible values of k_1 is also discrete by Proposition 3.1. ■

The rest of the proof of Theorem 2.1 is a (partially standard) argument of reducing a general metric to a scalar metric by introducing isothermic coordinates. This is done in Section 6.

4. PROOF OF THEOREM 3.3

Let

$$p(z) = z^n + a_{n-1}z^{n-1} + \dots + a_0$$

be a monic polynomial with roots z_1, \dots, z_n . The *discriminant* of p is defined as

$$\Delta(p) = \prod_{1 \leq i < j \leq n} (z_i - z_j)^2.$$

It is clear that $\Delta(p)$ vanishes if and only if p has roots of multiplicity greater than or equal to 2. It is well known (see, for example, [20, Section 5.9]) that $\Delta(p)$ is a polynomial function of the coefficients a_0, \dots, a_{n-1} .

Lemma 4.1. *Let \mathcal{C} be a simple closed contour in \mathbb{C} , and $\{T(z), z \in \mathcal{D}\}$ be an operator family of type A in a Hilbert space H analytic in a simply connected domain $\mathcal{D} \subset \mathbb{C}$. Suppose that the spectra of $T(z)$ within \mathcal{C} are discrete and finite for all $z \in \mathcal{D}$ and $\sigma(T(z)) \cap \mathcal{C} = \emptyset$ for all $z \in \mathcal{D}$. Then the set*

$$\{z \in \mathcal{D}: T(z) \text{ has at least one degenerate eigenvalue inside of } \mathcal{C}\}$$

is a zero set of a function analytic in \mathcal{D} , and hence either coincides with \mathcal{D} or is discrete in \mathcal{D} .

Proof. Let

$$P(z) := -\frac{1}{2\pi i} \int_{\mathcal{C}} (T(z) - \varkappa I)^{-1} d\varkappa$$

be the Riesz projection. By assumption, $n := \text{rank } P(z) = \text{const} < +\infty$, and $P(z)$ is analytic in \mathcal{D} . The results of [7, VII.1.3] imply that there exists an analytic in \mathcal{D} bounded operator-valued function $U: \mathcal{D} \rightarrow B(H)$ such that $U(\cdot)^{-1}$ is also analytic in \mathcal{D} and $P(z) = U(z)P(z_0)U(z)^{-1}$. Take

$$T_0(z) := U(z)^{-1}T(z)U(z) \Big|_{\text{ran } P(z_0)}.$$

The family $T_0(z)$ is an analytic operator family acting in a fixed finite-dimensional space that has the same eigenvalues and multiplicities as $T(z)$ restricted to $\text{ran } P(z)$. The monic polynomial $p_z(\varkappa) = (-1)^n \det(T_0(z) - \varkappa)$ is the characteristic polynomial of $T_0(z)$ and has the coefficients analytic in \mathcal{D} (in the variable z). Hence, its discriminant $\Delta(p_z)$ is also an analytic function in \mathcal{D} vanishing if and only if $T_0(z)$ (and, as a consequence, $T(z)$) has degenerate eigenvalues inside of \mathcal{C} . ■

Recall that we had a special choice of basis in Γ' ,

$$b'_1 = \alpha e_1, \quad b'_2 = \beta e_1 + e_2.$$

Let also

$$k = k_1 e_1 + k_2 e_2, \quad k_1 = r_1 + il_1, \quad k_2 = r_2 + il_2.$$

The following two theorems are the main technical statements of the paper. We postpone the proofs to the next section.

Theorem 4.2. *There exist constants $C = C(A, V, \omega)$ and $C_1 = C_1(A, V, \omega) \in 2\pi\mathbb{Z}$ such that for any $\delta > 0$ the operator $H(k)$ defined in (3.1) is invertible and satisfies*

$$\|H(k)^{-1}\| \leq \frac{C}{|l_1| \delta^2}$$

provided that $\text{dist}(r_2, 2\pi\mathbb{Z}) \geq \delta$, $l_1 \in 2\pi\mathbb{Z}$, $|l_1| \geq C_1$. As a consequence, the horizontal lines $\text{Im } k_1 = \pm C_1$ have empty intersection with $\sigma(T_1(k_2))$.

Without loss of generality, one can assume $\lambda = 0$ by choosing a different V . In the sequel, we will make this assumption and drop λ from the notation for T_1 , that is, $T_1(k_2) := T_1(k_2, 0)$.

Theorem 4.3. *There exists a constant $l = l(A, V, \omega) \in 2\pi\mathbb{Z}$ such that, for all $n \in 2\pi\mathbb{Z}$, the spectrum of $T_1(k_2)$ is simple for $k_2 = \frac{\pi}{2} + n + i\left(\frac{\pi}{2} + l\right)\alpha$.*

Proof of Theorem 3.3. Assume the contrary, i. e. that the set of $k_2 \in \mathbb{R}$ for which $T_1(k_2)$ has real degenerate eigenvalues has a limit point $k_2^{(0)}$. Let us consider two cases.

Case 1. Suppose that $\text{dist}(k_2^{(0)}, 2\pi\mathbb{Z}) > 0$. Take $\delta = \min\{\pi/2, \text{dist}(k_2^{(0)}, 2\pi\mathbb{Z})\}$. There exists a single $n \in 2\pi\mathbb{Z}$ such that $k_2^{(0)} \in [n + \delta, n + 2\pi - \delta]$. Let \mathcal{C}_0 be a path in the k_2 -plane starting at

$k_2^{(0)}$, then going straight towards the point $\frac{\pi}{2} + n$, and then going vertically towards the point $k_2^{(1)} := \frac{\pi}{2} + n + i\left(\frac{\pi}{2} + l\right)\alpha$ from Theorem 4.3.

The points $k_2 \in \mathcal{C}_0$ satisfy the assumptions of Theorem 4.2. Let us consider the eigenvalues of $T_1(k_2)$ lying within the strip $|\operatorname{Im} k_1| < C_1$, where C_1 is the constant from Theorem 4.2. They form a discrete $2\pi\alpha$ -periodic set. For each $k_2 \in \mathcal{C}_0$ there exists a point $r(k_2) \in \mathbb{R}$ which is *not* a real part of any of these eigenvalues. Moreover, by continuity arguments, this also holds in a small (complex) neighbourhood of k_2 . Let us cover \mathcal{C}_0 by a finite number of these neighbourhoods \mathcal{D}_j , $j = 1, \dots, p$, so that $k_2^{(0)} \in \mathcal{D}_1$ and $k_2^{(1)} \in \mathcal{D}_p$ and denote the corresponding values of $r(k_2)$ by r_j . For each j , denote by \mathcal{C}_j the boundary of the following rectangle:

$$r_j < \operatorname{Re} k_1 < r_j + 2\pi\alpha, \quad -C_1 < \operatorname{Im} k_1 < C_1.$$

Informally speaking, each rectangle contains all eigenvalues that we are interested in: they are initially on the real line, they cannot cross the lines $\operatorname{Im} k_1 = \pm C_1$, and the pictures to the right and to the left copy the picture in the rectangle due to periodicity.

Let us apply Lemma 4.1 to each of the domains \mathcal{D}_j and contours \mathcal{C}_j . Due to Theorem 4.3, the spectrum of $T_1(k_2^{(1)})$ is simple, and hence the set of “degenerate” k_2 should be discrete in a neighbourhood \mathcal{D}_p of $k_2^{(1)}$. By the standard arguments of analytic continuation, it should also be discrete in every neighbourhood $\mathcal{D}_1, \dots, \mathcal{D}_p$. However, since $k_2^{(0)} \in \mathcal{D}_1$, it is not discrete in \mathcal{D}_1 , which is a contradiction.

Case 2. Suppose that $k_2^{(0)} \in 2\pi\mathbb{Z}$. The set of *real* eigenvalues of $T_1(k_2^{(0)})$ is, again, discrete and $2\pi\alpha$ -periodic. Let us surround the eigenvalues on one period by a contour \mathcal{C} not containing any other eigenvalues. In a small neighbourhood \mathcal{D}_0 of $k_2^{(0)}$, these eigenvalues still stay within \mathcal{C} . Apply Lemma 4.1 to \mathcal{C} and \mathcal{D}_0 . Again, since the set of “degenerate” values of k_2 is not discrete in \mathcal{D}_0 , it should coincide with \mathcal{D}_0 , and hence there exists at least one more point with the same property that belongs to $\mathbb{R} \setminus 2\pi\mathbb{Z}$, and thus the situation reduces to Case 1. ■

5. PROOFS OF THEOREMS 4.2, 4.3

Let us start from recalling some notation introduced above,

$$b'_1 = \alpha e_1, \quad b'_2 = \beta e_1 + e_2, \quad \alpha, \beta \in \mathbb{R};$$

$$k = k_1 e_1 + k_2 e_2, \quad k_1 = r_1 + i l_1, \quad k_2 = r_2 + i l_2, \quad r_1, r_2, l_1, l_2 \in \mathbb{R}.$$

In this section, we will emphasize the dependence of H on g, A, V and use the notation $H(k; g, A, V)$. Consider the free operator $H_0(k) := H(k; \mathbf{1}, 0, 0)$. Its eigenfunctions are of the form

$$\exp\{im \cdot x\} = \exp\{i(m_1 b'_1 + m_2 b'_2) \cdot (x_1 e_1 + x_2 e_2)\} = \exp\{i(\alpha m_1 + \beta m_2)x_1 + m_2 x_2\},$$

$$m = m_1 b'_1 + m_2 b'_2 \in \Gamma', \quad m_1, m_2 \in 2\pi\mathbb{Z},$$

and

$$H_0(k) \exp\{im \cdot x\} = ((-i\partial_1 + k_1)^2 + (-i\partial_2 + k_2)^2) \exp\{im \cdot x\} = h_m(k) \exp\{im \cdot x\},$$

where $h_m(k)$ is the symbol of $H_0(k)$:

$$h_m(k) = (\alpha m_1 + \beta m_2 + k_1)^2 + (m_2 + k_2)^2 = q_m^+(k) q_m^-(k),$$

$$q_m^\pm(k) = \alpha m_1 + \beta m_2 + r_1 \mp l_2 + i(l_1 \pm m_2 \pm r_2).$$

Let also $Q^\pm(k)$ be the operators with symbols $q_m^\pm(k)$ respectively, so that $H_0(k) = Q^+(k)Q^-(k)$. Suppose that the magnetic potential A satisfies (2.3). Then there exists a Γ -periodic scalar function $\varphi \in C_{\text{per}}^2(\Omega)$ such that

$$(5.1) \quad (\nabla\varphi)(x) = A_2(x)e_1 - A_1(x)e_2, \quad \int_{\Omega} \varphi(x) dx = 0, \quad \|\varphi\|_{C^2(\Omega)} \leq C\|A\|_{C^1(\Omega)}.$$

Let also

$$B(x) = \partial_1 A_2(x) - \partial_2 A_1(x), \quad w(x) := e^{-2\varphi(x)}.$$

The operator $H(k; \mathbf{1}, A, B)$ is called *the Pauli operator* (more precisely, a block of the Pauli operator). The following is proved in [2] and allows us to reduce the case of the magnetic potential, essentially, to the case of the free operator.

Proposition 5.1. *Under the above assumptions, if $Q^\pm(k)$ are invertible, then $H(k; \mathbf{1}, A, B)$ is also invertible, and*

$$(5.2) \quad H(k; \mathbf{1}, A, B)^{-1} = e^\varphi Q^-(k)^{-1} e^{-2\varphi} Q^+(k)^{-1} e^\varphi = e^{\varphi(x)} H_0(k)^{-1} \{e^{-\varphi} + (-i\partial_1 w + \partial_2 w) Q^+(k)^{-1} e^\varphi\}.$$

The following proposition can also be easily verified, see [3]. It will be used to reduce the case of a scalar metric $g = \omega^2 \mathbf{1}$ to the case $g = \mathbf{1}$.

Proposition 5.2. *Suppose that $\omega \in C_{\text{per}}^2(\Omega)$, $V \in L^\infty(\Omega)$, $A \in C_{\text{per}}^1(\Omega)$. Then*

$$(5.3) \quad H(k; \omega^2 \mathbf{1}, A, V) = \omega H(k; \mathbf{1}, A, \omega^{-2} V + \omega^{-1} \Delta \omega) \omega,$$

$$(5.4) \quad \omega H(k; \mathbf{1}, A, V) \omega = H(k; \omega^2 \mathbf{1}, A, \omega^2 V - \omega \Delta \omega).$$

Proof of Theorem 4.2. Suppose that $\text{dist}(r_2, 2\pi\mathbb{Z}) = \delta$. Since $l_1 \pm m_2 \in 2\pi\mathbb{Z}$, we have $|q_m^\pm(k)| \geq \delta$. In addition, $\text{Im } q_m^+(k) + \text{Im } q_m^-(k) = 2l_1$, and hence we either have $|q_m^+(k)| \geq |l_1|$ or $|q_m^-(k)| \geq |l_1|$. Combining these estimates, we obtain $|h_m(k)| \geq |l_1|\delta$, and

$$(5.5) \quad \|H_0(k)^{-1}\| \leq \frac{1}{|l_1|\delta}, \quad \|Q^+(k)^{-1}\| \leq \frac{1}{\delta},$$

which completes the proof for $A = 0$, $V = 0$, $\omega = 1$. If $A \neq 0$ and $V(x) = B(x)$, then, from (5.2) and (5.5), we get

$$(5.6) \quad \|H(k; \mathbf{1}, A, B)^{-1}\| \leq \frac{C_1}{|l_1|\delta^2},$$

where C_1 depends on A via w and φ . The standard Neumann series arguments imply that the bound (5.6) holds for an arbitrary $V \in L^\infty(\Omega)$ (with a different C_1) for sufficiently large l_1 , say,

$$|l_1| \geq \frac{2\|V - B\|_{L^\infty(\Omega)} C_1}{\delta^2}.$$

The case of arbitrary ω follows from Proposition 5.2. ■

We now make some preparations for the proof of Theorem 4.3. Fix k_2 as in the formulation of the theorem, so that

$$(5.7) \quad r_2 = \frac{\pi}{2} + n, \quad l_2 = \left(\frac{\pi}{2} + l\right) \alpha, \quad l, n \in 2\pi\mathbb{Z}.$$

For these k_2 , define

$$\Sigma_n := \{k_1 \in \mathbb{C} : h_m(k_1, k_2) = 0 \text{ for some } m_1, m_2 \in 2\pi\mathbb{Z}\}.$$

In other words, it is the set of k_1 for which $H_0(k_1, k_2)$ is not invertible. A simple computation shows that Σ_n consists of points $r_1 + il_1$ of the following form:

$$(5.8) \quad \begin{cases} r_1 = -\alpha m_1 - \beta m_2 \mp (\frac{\pi}{2} + l) \alpha \\ l_1 = \pm (\frac{\pi}{2} + n + m_2) \end{cases}, \quad m_1, m_2 \in 2\pi\mathbb{Z}.$$

Since one can replace the variables m_1 by $m_1 + l$, one can see that *the set Σ_n does not depend on l .*

Let us describe the set Σ_n in more detail. First of all, it is easy to see that different values of (m_1, m_2) give different points of Σ_n , as m_2 and the signs are uniquely determined by the value of l_1 , and m_1 is determined by r_1 afterwards. Next, the set Σ_n lies on the union of horizontal lines $\text{Im } k_1 \in \pi/2 + \pi\mathbb{Z}$. On each line, it is a sequence of equally spaced points with the spacings $2\pi\alpha$.

We will also need another set G_n defined by

$$(5.9) \quad G_n := (\mathbb{R} + i\pi\mathbb{Z}) \cup \bigcup_{z \in \Sigma_n} \left(z + \pi\alpha + i \left[-\frac{\pi}{2}, \frac{\pi}{2} \right] \right).$$

The set G_n consists of horizontal lines $\text{Im } k_1 \in \pi\mathbb{Z}$ separating the horizontal lines of Σ_n . In addition, for each point of Σ_n , we include a vertical line segment of the length π separating this point from the next point of Σ_n lying on the same line. One can imagine G_n as a “brick wall” consisting of rectangles such that there is exactly one element of Σ_n inside of each rectangle.

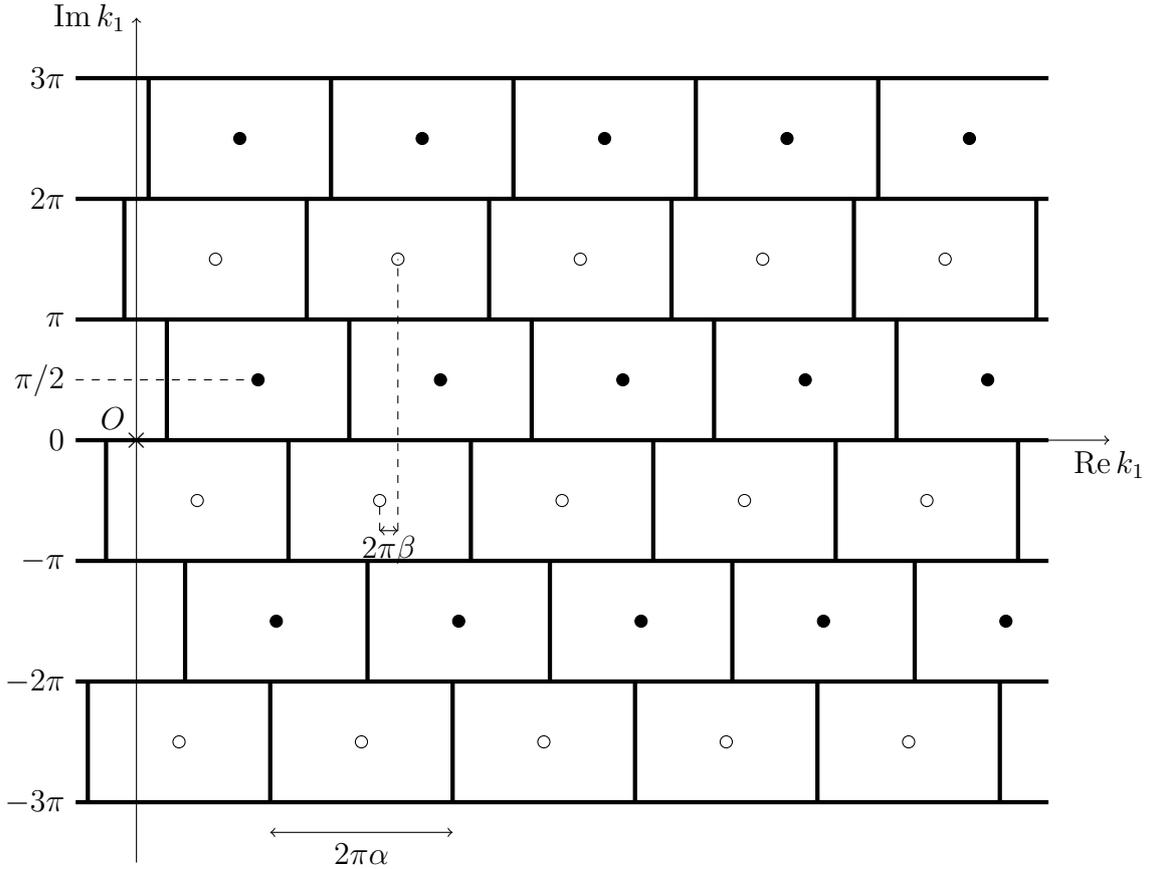


FIGURE 1. The sets Σ_n and G_n .

On Figure 1, an example of Σ_n and G_n is shown for $n = 0$, $\alpha = 0.75$, $\beta = 0.075$. The set G_n is represented by thick lines, and the locations of points of Σ_n are indicated by black and white circles, corresponding to the upper or lower choice of signs in (5.8), respectively.

Lemma 5.3. *Suppose that $k_1 \in G_n$, $k_2 = \frac{\pi}{2} + n + i\left(\frac{\pi}{2} + l\right)\alpha$, where $l, n \in 2\pi\mathbb{Z}$. Then*

$$|h_m(k)| \geq C|l|$$

uniformly in $m_1, m_2 \in 2\pi\mathbb{Z}$.

Proof. Since $|\operatorname{Re} q_m^+(k) - \operatorname{Re} q_m^-(k)| = 2|l_2| \geq C|l|$, we have for each m either $|q_m^+(k)| \geq \frac{1}{2}C|l|$ or $|q_m^-(k)| \geq \frac{1}{2}C|l|$. On the other hand, both $|q_m^+(k)|$ and $|q_m^-(k)|$ are distances from k_1 to a certain point of Σ_n , which is bounded from below by a positive constant,

$$(5.10) \quad |q_m^\pm(k)| \geq \operatorname{dist}(k_1, \Sigma_n) \geq \operatorname{dist}(G_n, \Sigma_n) = \min \left\{ \frac{\pi}{2}, \pi\alpha \right\}.$$

The combination of these estimates completes the proof of the lemma. ■

Remark 5.4. Lemma 5.3 is the main ingredient of the proof that relies on the assumption $d = 2$. In $d \geq 3$, one cannot construct a set G_n with similar properties and constant size of the bricks.

Corollary 5.5. *Under the assumptions of Lemma 5.3, there exists $L_0(A, V, \omega) > 0$ such that, if $|l| > L_0(\omega, A, V)$, then*

$$(5.11) \quad \|H(k; \omega^2 \mathbf{1}, A, V)^{-1}\| \leq \frac{C(\omega, A, V)}{|l|},$$

where the constants C and L_0 depend only on $\|A\|_{C^1(\Omega)}$, $\|V\|_{L^\infty(\Omega)}$, $\|\omega\|_{C^2(\Omega)}$ and on the constant m_g from (2.4).

Proof. From Proposition 5.2, we have

$$\|H(k; \omega^2 \mathbf{1}, A, V)^{-1}\| \leq m_g^{-2} \|H(k; \mathbf{1}, A, V_\omega)^{-1}\|,$$

where

$$\|V_\omega\|_{L^\infty(\Omega)} = \|\omega^{-2}V + \omega^{-1}\Delta\omega\|_{L^\infty(\Omega)} \leq m_g^{-2}\|V\|_{L^\infty(\Omega)} + m_g^{-1}\|\omega\|_{C^2(\Omega)}.$$

From (5.2), (5.1), Lemma 5.3, and (5.10), we have

$$\|H(k; \mathbf{1}, A, B)^{-1}\| \leq C(A) \|H_0(k)^{-1}\| \leq \frac{C_1(A)}{|l|},$$

where $C(A)$, $C_1(A)$ depend only on $\|A\|_{C^1(\Omega)}$. Since $\|B\|_{L^\infty(\Omega)} \leq 2\|A\|_{C^1(\Omega)}$, we can use the same Neumann series argument as in the proof of Theorem 4.2 to replace B by V_ω . ■

Proof of Theorem 4.3. Denote by $T_\mu(k_2)$ the operator $T_1(k_2)$ with V , A , ω replaced by μV , μA and $\mu\omega + (1 - \mu)$ respectively. It is a one-parametric family connecting the “free” operator $T_0(k_2)$ with $T_1(k_2)$.

It is easy to see that $\sigma(T_0(k_2)) = \Sigma_n$, because Σ_n is exactly the set of $k_1 \in \mathbb{C}$ for which the symbol of $H_0(k)$ is not invertible. Moreover, an easy computation shows that, for each $k_1 \in \Sigma_n$, the corresponding eigenspace is one-dimensional and is spanned by $\begin{pmatrix} e^{im \cdot x} \\ k_1 e^{im \cdot x} \end{pmatrix}$, where m is determined by k_1 via (5.8). Note that each value of m appears twice (for two different values of k_1) because of two possible signs. Hence, the total collection of eigenvectors spans $H_{\text{per}}^1(\Omega) \oplus L^2(\Omega)$, so there are no Jordan cells and *the spectrum of $T_0(k_2)$ is simple*.

It remains to prove that $T_1(k_2)$ also has simple spectrum. Consider the Riesz projection of $T_\mu(k_2)$ with respect to the boundary of some rectangle of G_n . For $\mu = 0$, the rectangle contains exactly one simple eigenvalue, and the range of the projection has dimension 1. Let us increase μ . The only way for the dimension of the range to change is to have an eigenvalue of $T_\mu(k_2)$ approach the set G . This, however, is impossible for $\mu \in [0, 1]$ due to Corollary 5.5, and hence the eigenvalues of $T_1(k_2)$ stay simple. ■

Remark 5.6. The proof of Theorem 4.3 is based on the ideas of [6, Section VI].

6. THE CASE OF VARIABLE METRIC

In this section we show how to reduce the case of an operator with arbitrary metric g satisfying (2.4) to the case of the scalar metric. The technical difference with standard arguments such as in [17] is that we need to keep track of the quasimomentum in order to ensure that it is transformed linearly. This is done by an additional “gauge transformation”. The following proposition establishes the existence of *global isometric coordinates* in which the metric g becomes scalar. See [12, Proposition 18] for the proof.

Proposition 6.1. *Suppose that g satisfies (2.4). Then there exists a basis b_1^*, b_2^* of \mathbb{R}^2 and a one-to-one map $\Psi: \mathbb{R}^2 \rightarrow \mathbb{R}^2$, $\Psi \in C^3(\mathbb{R}^2)$, $\det \Psi'(x) \neq 0$, and a scalar such that*

$$\Psi(0) = 0, \quad \Psi(x + n_1 b_1 + n_2 b_2) = \Psi(x) + n_1 b_1^* + n_2 b_2^*, \quad \forall n_1, n_2 \in \mathbb{Z},$$

and

$$(6.1) \quad |\det \Psi'(x)|^{-1} \Psi'(x) g(x) \Psi'(x)^t = \omega^2(\Psi(x)) \mathbf{1},$$

where $\omega \in C^2(\mathbb{R}^2)$ is a Γ_* -periodic strictly positive scalar function.

Let us introduce some notation. Suppose that the operator $H(g, A, V)$ satisfies the assumptions of Theorem 2.1. Let Ψ be the transformation obtained from Proposition 6.1. Denote by $T_*: \mathbb{R}^2 \rightarrow \mathbb{R}^2$ the linear transformation defined by $T_*(b_1) = b_1^*$, $T_*(b_2) = b_2^*$. The transformation T_* , as well as the map Ψ , transforms the lattice Γ into the new lattice Γ_* with the basis vectors b_1^*, b_2^* . Let also

$$y = \Psi(x), \quad A_*(y) = (\Psi'(x)^{-1})^t A(x), \quad V_*(y) = \psi_*(y)^{-2} V(x), \quad \psi_*(y) = |\det \Psi'(x)|^{1/2}.$$

Let also

$$\Omega_\Psi = \Psi(\Omega), \quad \Omega_* = \{y_1 b_1^* + y_2 b_2^*, \quad y_1, y_2 \in [0, 1)\}.$$

Note that both Ω_* and Ω_Ψ are fundamental domains of Γ_* , and there is a natural correspondence between $L^2(\Omega_*)$ and $L^2(\Omega_\Psi)$, as both can be identified with \mathbb{R}^d/Γ_* .

Lemma 6.2. *In the above notation, let $\Phi: L^2(\Omega) \rightarrow L^2(\Omega_*)$ be the unitary operator of change of variables:*

$$u(x) = \psi_*(y)(\Phi u)(y), \quad y = \Psi(x),$$

where u is considered as an element of $L^2(\Omega_*)$. Then

$$\Phi H(0; g, A, V) \Phi^{-1} = \psi_* H(0; \omega^2 \mathbf{1}, A_*, V_*) \psi_*.$$

Proof. Let $v = \Phi u$, and let us extend it Γ_* -periodically into \mathbb{R}^d . Then, due to (6.1) and the change of variable rule, the quadratic form of the left hand side applied to v is equal to

$$\begin{aligned} & (H(0; g, A, V) \Phi^{-1} v, \Phi^{-1} v)_{L^2(\Omega)} = (H(0; g, A, V) u, u)_{L^2(\Omega)} = \\ & = \int_{\Omega} \langle g(x)(-i\nabla_x - A(x))u(x), (-i\nabla_x - A(x))u(x) \rangle dx + \int_{\Omega} V(x)|u(x)|^2 dx \end{aligned}$$

$$\begin{aligned}
&= \int_{\Omega_{\Psi}} \langle \omega^2(y)(-i\nabla_y - A_*(y))\psi_*(y)v(y), (-i\nabla_y - A_*(y))\psi_*(y)v(y) \rangle dy + \int_{\Omega_{\Psi}} V_*(y)\psi_*(y)^2|v(y)|^2 dy = \\
&= \int_{\Omega_*} \langle \omega^2(y)(-i\nabla_y - A_*(y))\psi_*(y)v(y), (-i\nabla_y - A_*(y))\psi_*(y)v(y) \rangle dy + \int_{\Omega_*} V_*(y)\psi_*(y)^2|v(y)|^2 dy = \\
&= (H(0; \omega^2 \mathbf{1}, A_*, V_*)\psi_* v, \psi_* v)_{L^2(\Omega_*)}. \blacksquare
\end{aligned}$$

Theorem 6.3. *Suppose that $k \in \mathbb{R}^2$. Under the assumptions of Theorem 2.1, the operator $H(k; g, A, V)$ is unitarily equivalent to the operator*

$$(6.2) \quad H((T_*^{-1})^t k, \omega^2 \psi_*^2 \mathbf{1}, A_*, \psi_*^2 V_* + \psi_*^2 \omega \Delta \omega - \psi_* \omega \Delta (\psi_* \omega))$$

acting in $L^2(\Omega_*)$, where Ω_* is the elementary cell of Γ_* .

Proof. We will perform the required unitary transformation in several steps. First, let us note that $H(k; g, A, V) = H(0; g, A - k, V)$. Consider the unitary transformation $u(x) = e^{i\alpha(x)}v(x)$, where $\alpha \in C_{\text{per}}^1(\Omega)$. Under this transformation, the operator $H(k; g, A, V)$ becomes $H(0; g, A - k - \nabla\alpha, V)$. Take $\alpha(x) = k(T_*^{-1}\Psi(x) - x)$. This function is Γ -periodic, and

$$(\nabla\alpha)(x) = \Psi'(x)^t (T_*^{-1})^t k - k.$$

Hence, the operator $H(k; g, A, V)$ is unitarily equivalent to $H(0, g, A - \Psi'(x)^t (T_*^{-1})^t k, V)$, which, by Lemma 6.2, is equivalent to

$$\psi_* H(0, \omega^2 \mathbf{1}, A_* - (T_*^{-1})^t k, V_*) \psi_* = \psi_* H((T_*^{-1})^t k, \omega^2 \mathbf{1}, A_*, V_*) \psi_*.$$

Applying (5.3) and then (5.4), we ultimately obtain

$$\begin{aligned}
\psi_* H((T_*^{-1})^t k, \omega^2 \mathbf{1}, A_*, V_*) \psi_* &= \omega \psi_* H((T_*^{-1})^t k, \mathbf{1}, A_*, \omega^{-2} V_* + \omega^{-1} \Delta \omega) \omega \psi_* = \\
&= H((T_*^{-1})^t k, \omega^2 \psi_*^2 \mathbf{1}, A_*, \psi_*^2 V_* + \psi_*^2 \omega \Delta \omega - \psi_* \omega \Delta (\psi_* \omega)). \blacksquare
\end{aligned}$$

This completes the proof of Theorem 2.1, because its statement has already been established for the operators (6.2), and the operator families $H(k; g, A, V)$ and (6.2) have the same band functions up to a linear transformation of k .

7. AN EXAMPLE OF DEGENERATE BAND EDGE IN THE DISCRETE CASE

Consider the discrete Schrödinger operator $H = \mathcal{D} + V$ in $l^2(\mathbb{Z}^2)$, where

$$(\mathcal{D}u)_n = \frac{1}{2} (u_{n+e_1} + u_{n-e_1} + u_{n+e_2} + u_{n-e_2}), \quad n \in \mathbb{Z}^2,$$

is the discrete Laplace operator, and V is the operator of multiplication by the potential given by

$$(Vu)_n = \begin{cases} v_0 u_n, & \text{if } (n_1 + n_2) \text{ is even,} \\ v_1 u_n, & \text{if } (n_1 + n_2) \text{ is odd;} \end{cases}$$

the real numbers v_0 and v_1 are fixed. In other words, the lattice is formed by two different types of atoms placed in a chess-like order, and V is periodic with respect to the lattice spanned by $\{2e_1, e_1 + e_2\}$. The corresponding Floquet-Bloch transform

$$F : l^2(\mathbb{Z}^2) \rightarrow L^2(\tilde{\mathcal{O}} \times \{0; 1\})$$

is given by

$$(Fu)(k; m) = \frac{1}{\pi\sqrt{2}} \sum_{n_1+n_2 \equiv m \pmod{2}} e^{-ikn} u_n.$$

Here $k \in \tilde{\mathcal{O}} = \{k \in \mathbb{R}^2 : |k_1 + k_2| < \pi\}$, $m = 0$ or $m = 1$; the operator F is unitary. It is easy to see that

$$FHF^* = \int_{\tilde{\mathcal{O}}}^{\oplus} H(k) dk,$$

where $H(k)$ is a self-adjoint operator in \mathbb{C}^2 ,

$$H(k) = \begin{pmatrix} v_0 & \cos k_1 + \cos k_2 \\ \cos k_1 + \cos k_2 & v_1 \end{pmatrix}.$$

Eigenvalues of this matrix are

$$\lambda_{\pm}(k) = \frac{v_0 + v_1}{2} \pm \sqrt{\left(\frac{v_0 - v_1}{2}\right)^2 + (\cos k_1 + \cos k_2)^2},$$

from which it follows that

$$\min \lambda_- = \frac{v_0 + v_1}{2} - \sqrt{\left(\frac{v_0 - v_1}{2}\right)^2 + 4}, \quad \max \lambda_- = \min(v_0, v_1),$$

$$\min \lambda_+ = \max(v_0, v_1), \quad \max \lambda_+ = \frac{v_0 + v_1}{2} + \sqrt{\left(\frac{v_0 - v_1}{2}\right)^2 + 4}.$$

So, the spectrum of the operator H consists of two zones separated by a gap, whenever $v_0 \neq v_1$.

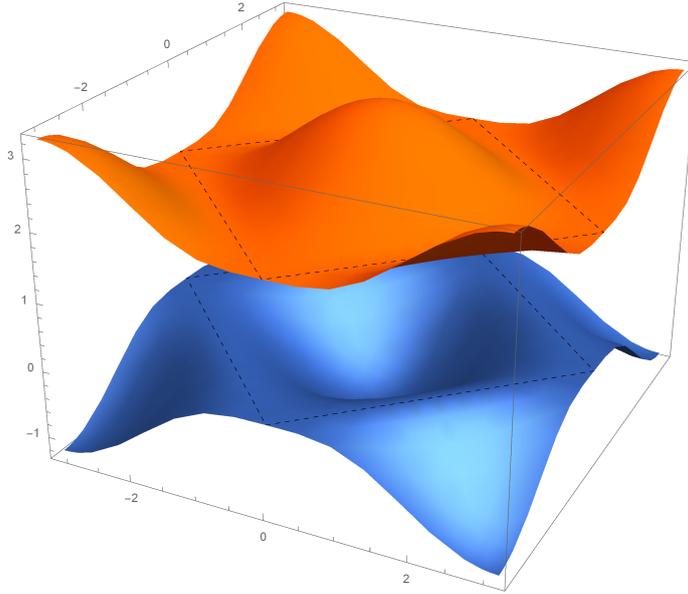


FIGURE 2. The band functions $\lambda_+(k)$ and $\lambda_-(k)$.

The edges of this gap (v_0 and v_1 respectively) are attained on the set

$$\{k \in \mathbb{R}^2 : \cos k_1 + \cos k_2 = 0\} = \{k \in \mathbb{R}^2 : k_1 \pm k_2 = (2p + 1)\pi\}_{p \in \mathbb{Z}},$$

which is a countable union of straight lines. Figure 2 shows the graphs of $\lambda_{\pm}(\cdot)$ for $v_0 = 0$, $v_1 = 2$, with the dashed lines indicating the level sets at the edges of the gap $[0, 2]$.

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