

EDGE STATES FOR TIGHT-BINDING OPERATORS WITH SOFT WALLS

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ABSTRACT. We study one- and two-dimensional periodic tight-binding models under the presence of a potential that grows to infinity in one direction, hence preventing the particles to escape in this direction (the soft wall). We prove that a spectral flow appears in these corresponding edge models, as the wall is shifted. We identify this flow as a number of Bloch bands, and provide a lower bound for the number of edge states appearing in such models.

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1. INTRODUCTION

The goal of this paper is to study *edge states* in terminated periodic structures described by tight-binding (TB) Hamiltonians. Such TB operators are extensively studied in condensed matter, as they provide simple models which correctly reproduce the physics of more complex continuous

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ones (represented *e.g.* by continuous Schrödinger operators). This research is motivated by models from solid state physics such as the one-dimensional Su-Schrieffer-Heeger (SSH) chain [30] and the two-dimensional Wallace model for graphene [32]. Indeed, it is known for these models that edge states may appear when these periodic systems are restricted to a halfspace. For the Wallace model for instance, the presence of these edge states depends strongly on the direction of the cut. Notable examples are the *zigzag cut*, where a flat band of edge modes appear, and the *armchair cut*, where no edge states appear, see [1, 25, 7, 11, 9, 10]. Even in the simple one-dimensional SSH model, an edge state appears or disappears depending on which of the nonequivalent *bonds* is cut. In these one-dimensional systems, the topological versus *trivial* nature of experimentally observed edge states is still a topic of hot debate (see *e.g.* [26] for theoretical considerations and [5] for recent experimental results) ever since the first reports of Majorana fermions in superconducting wires [6, 24].

In the present article, we give a framework to study the appearance of edge modes in general TB models arising in a wide variety of physical situations, such as graphene sheets, superconducting wires or optical lattices. However, instead of working with *hard truncations* (Dirichlet boundary conditions), as it is usually done in numerical simulations, we are interested in edge modes that arise from the lattice termination by a *soft wall*, that is, a continuous potential barrier that impedes the propagation in one halfspace. The main reason is that one cannot translate properly a *hard cut* in TB models. To illustrate the problem, imagine a TB problem on the line \mathbb{Z} , with the presence of a hard wall whose position is parametrized by $t \in \mathbb{R}$, with the convention that one deletes all sites on the left of t . Then, when t varies in an interval of the form $(n-1, n)$, nothing changes, but when t crosses the site n , the corresponding Hilbert space suddenly switches from $\ell^2(\{n, n+1, \dots\})$ to $\ell^2(\{n+1, n+2, \dots\})$. The corresponding operators are not continuous in t , which makes this case difficult to study. Note that, for some experimental realizations of periodic systems, confinement by a smooth potential instead of a sharp lattice termination is easily achieved. Numerical results on the effect of soft confinement in different configurations can be found for instance in [4, 14, 15].

We prove the appearance of a spectral flow in the gaps of the essential spectrum as the soft wall is shifted, and relate this flow with a number of Bloch bands (see Theorem 1.1). In particular, our result implies the presence of edge states for *many* values of t . Surprisingly, this spectral flow is independent of the shape of the wall. However, in the case where the soft wall varies slowly with respect to the lattice constant, we can prove that edge states always appear, for *all* values of t , regardless of the topological properties of the material (see Theorem 1.3 below).

When studying the analogue of this problem for continuous models, that is for Schrödinger operators with periodic potentials in \mathbb{R} or \mathbb{R}^2 , one can use the spectral flow to study the effect of hard truncations, modelled by a Dirichlet boundary condition along a line parametrized by a translation parameter t (the cut). These models have been studied in [16, 17, 18], where it is proved that a spectral flow appears as the cut is translated. In addition, this spectral flow can be computed explicitly, and is related to a number of Bloch bands of the initial bulk operator. The results of the present paper are the discrete analogue of these, although the techniques of proof are rather different.

In the two-dimensional case, we also prove that numerous edge modes must appear when one cuts such materials with a commensurate angle having large numerators/denominators. Actually, following the lines of [17], one could prove that *all bulk gaps are filled with edge spectrum* in the incommensurate case (although we do not provide a full proof here, as it is similar to the one in [17]).

Let us give a short description of our main result in the one-dimensional setting. We consider a general TB bulk operator H acting on $L^2(\mathbb{Z}, \mathbb{C}^N)$, of the convolution form

$$\forall \Psi \in \ell^2(\mathbb{Z}, \mathbb{C}^N), \quad \forall n \in \mathbb{Z}, \quad (H\Psi)_n = \sum_{m \in \mathbb{Z}} h(m) \Psi_{n-m} =: (h * \Psi)_n$$

where for each $n \in \mathbb{Z}$, $h(n)$ is an $N \times N$ matrix such that $h^*(n) = h(-n)$. We assume throughout that $\sum_n \|h_n\|_{\text{op}} < \infty$, which guarantees the boundedness of the operator by Young's inequality (see Lemma 2.1 below). By taking a Fourier transform, the spectrum of H is purely essential, of the form

$$\sigma_{\text{bulk}} := \sigma(H) = \bigcup_{k \in \mathbb{R}} \sigma(H_k), \quad \text{with} \quad H_k := \sum_{m \in \mathbb{Z}} h(m) e^{-ikm}.$$

The map $k \mapsto H_k$ is 2π -periodic and analytic, and takes values in \mathcal{S}_N , the set of Hermitian $N \times N$ matrices. Let $\lambda_{1,k} \leq \dots \leq \lambda_{N,k}$ be the eigenvalues of H_k ranked in increasing order. By standard perturbation theory [23], for all $1 \leq j \leq N$, the map $k \mapsto \lambda_{j,k}$ is continuous and 2π -periodic. The j -th *Bloch band* is the image of this map, namely the interval $\bigcup_k \{\lambda_{j,k}\}$. The connected components of $\mathbb{R} \setminus \sigma_{\text{bulk}}$ are the *gaps* in the essential spectrum. For an energy $E \in \mathbb{R} \setminus \sigma_{\text{bulk}}$, we denote by $\mathcal{N}(E)$ the number of Bloch bands below E . It is the unique integer such that

$$\forall k \in [-\pi, \pi], \quad \lambda_{\mathcal{N}(E),k} < E < \lambda_{\mathcal{N}(E)+1,k},$$

with the convention that $\lambda_{0,k} = -\infty$ and $\lambda_{N+1,k} = +\infty$. Occasionally, when comparing several bulk operators, we will also write $\mathcal{N}_H(E)$.

We now perturb the bulk Hamiltonian by adding the wall potential. We fix a Lipschitz continuous function $w : \mathbb{R} \rightarrow \mathcal{S}_N$ satisfying

$$\forall v \in \mathbb{C}^N \setminus \{0\}, \quad \lim_{x \rightarrow -\infty} \langle v, w(x)v \rangle = +\infty \quad \text{and} \quad \lim_{x \rightarrow +\infty} \langle v, w(x)v \rangle = 0. \quad (1)$$

The first limit states that the lowest eigenvalue of $w(x)$ diverges to $+\infty$ as $x \rightarrow -\infty$, and the second that all entries of the matrix w converge to 0 as $x \rightarrow +\infty$. From w , we define the wall operator $W(t)$ acting on $\ell^2(\mathbb{Z}, \mathbb{C}^N)$ as the multiplication operator

$$\forall \Psi \in \ell^2(\mathbb{Z}, \mathbb{C}^N), \quad (W(t)\Psi)_n := w(n-t)\Psi_n.$$

The parameter $t \in \mathbb{R}$ indicates a shift in the position of the wall. Our goal is to study the family of *edge operators* $t \mapsto H^\sharp(t)$ defined by

$$H^\sharp(t) := H + W(t), \quad \text{specifically} \quad (H^\sharp(t)\Psi)_n = (h * \Psi)_n + w(n-t)\Psi_n.$$

It is not difficult to see that the family $t \mapsto H^\sharp(t)$ is 1-quasi-periodic, in the sense that $H^\sharp(t+1) = \tau_1^* H^\sharp(t) \tau_1$, where τ_1 is the usual translation operator $(\tau_1 \Psi)_n := \Psi_{n-1}$. We prove in Proposition 2.4 below that for all $t \in \mathbb{R}$, $H^\sharp(t)$ is self-adjoint with a domain independent of t , and that the essential spectrum of $H^\sharp(t)$ is also independent of t . However, some extra eigenvalues may appear in the essential gaps as t moves. For $E \in \mathbb{R} \setminus \sigma_{\text{bulk}}$, we denote by

$$\text{Sf}(H^\sharp(t), E, [0, 1])$$

the **spectral flow** of $t \mapsto H^\sharp(t)$ at energy E as t increases from 0 to 1. It counts the net number of eigenvalues of $t \mapsto H^\sharp(t)$ crossing the energy E downwards (see Appendix A for a precise definition, following [2, 27, 8]). Let us state our main result.

Theorem 1.1. *Let $w : \mathbb{R} \mapsto \mathcal{S}_N$ be a Lipschitz function satisfying (1). For all $E \in \mathbb{R} \setminus \sigma_{\text{bulk}}$, the energy E is in the essential gaps of all operators $H^\sharp(t)$, and*

$$\text{Sf}(H^\sharp(t), E, [0, 1]) = -\mathcal{N}(E),$$

where we recall that $\mathcal{N}(E)$ is the number of Bloch bands below E for the bulk-operator.

In particular, the spectral flow is independent of the precise expression for the soft-wall. A nonzero spectral flow implies that, at least for some values of $t \in \mathbb{R}$, the set $\sigma_{\text{edge}}(t) := \sigma(H^\sharp(t)) \setminus \sigma_{\text{bulk}}$, sometimes called the *edge spectrum*, is non empty. It only consists of eigenvalues. The corresponding eigenvectors are called *edge states*, and describe localized modes which are blocked by the wall on the left, and which cannot propagate in the medium on the right.

Remark 1.2. *The result is the discrete analogue to the one in [18], up to the minus sign. This is due to the fact that in the present article, the wall is moving to the right when t increases, which is the direction opposite to the one in [18]. In [17, 18] (see also [19]), one of us gave an interpretation of this result, that we called the **Grand Hilbert Hotel**, that might be useful. It is similar to the*

charge pumping *denomination of Thouless* [31]. Basically, we may think of each Bloch band as a hotel floor with an infinite number of rooms, each room occupied by one guest (or fermion). As t goes from 0 to 1, the wall is pushed on the right, deleting the leftmost rooms. A particle from the lowest band moves up to the second band, giving a spectral flow of -1 in the gap above the first band. Two particles cross the gap above the second band: one from the deleted leftmost room, and one to accommodate the new arrival from the first band, and so on.

In practice, one is often interested in the spectrum of $H^\sharp(t = t_0)$, that is for a single value of t . We have the following (see Section 2.3 for the proof).

Theorem 1.3. *Let $w : \mathbb{R} \mapsto \mathcal{S}_N$ be a soft-wall which is ν -Lipschitz, for some $\nu > 0$. If E belongs to an essential gap of H , then for all $t_0 \in \mathbb{R}$ the operator $H^\sharp(t_0)$ has at least $\mathcal{N}(E)$ eigenvalues in each interval of the form $(\lambda, \lambda + \nu]$ in this gap.*

In other words, the density of eigenvalues in the gap containing E is $\mathcal{N}(E)/\nu$. If ν is small, the potential W increases slowly to $+\infty$ on the left. It somehow acts as a local energy shift. It is therefore not so surprising that many eigenvalues appear in all gaps in this situation. On the other hand, if ν is very large, (imagine a situation where one approximates a hard cut by a sequence of soft wall with $\nu \rightarrow \infty$) then the spectral flow does not give information on the spectrum of $H^\sharp(t_0)$: it may or may not contain extra eigenvalues. Figure 3 below illustrates this situation for the SSH model.

Before we go on, let us recall that there are several ways to derive TB models from continuous ones. One approach, called the *strong binding limit*, is given in [12, 13, 28], and consists in studying the limit of continuous Schrödinger operators with a periodic potential, when the *wells* of the potential approach a delta-function centered on each atom. In this limit (similar to the semi-classical one), the wave-function Ψ is replaced by a discrete function giving the amplitude of Ψ associated to each atom. Another way to derive TB models is through the use of Wannier functions. In this case, one finds a countable set of functions (w_i) which are well-localized around the atoms (\mathbf{x}_i) , and which span the lowest part of the spectrum of the continuous Hamiltonian. A continuous wave-function $\Psi(x)$ is then approximated by the sum $\sum c_i w_i(x)$. Thanks to the localization of w_i , the value $c_i w_i(\mathbf{x}_i)$ can be interpreted as the value $\Psi(\mathbf{x}_i)$. The hopping transition between atoms i and j are then $t_{ij} = \langle w_i, H w_j \rangle$. We refer to [29, 20] for more details.

The paper is structured as follows. In Section 2, we prove some basic properties of one-dimensional Hamiltonians with and without soft walls. We explain how to reduce the problem to the somewhat easier case of periodic *Jacobi* operators and prove Theorem 1.1 assuming it holds for Jacobi operators. As an illustration of the general results we discuss the SSH chain in Section 2.4 and present numerical simulations of its spectrum. In Section 2.3, we give the proof of Theorem 1.3, again assuming the version of Theorem 1.1 for Jacobi operators.

The computation of the spectral flow for periodic Jacobi operators takes up the entire Section 3. This is the main technical part of the paper.

In Section 4, we explain how to extend our result in the two-dimensional setting. The main observation is that a 2d model, even cut by a (commensurate) soft-wall, is still periodic in the direction along the wall. After a Fourier transform in this direction, we are left with a family of one-dimensional models, indexed by the momentum in the direction along the wall. We prove in Theorem 4.5 that the greater the incommensurability of the cut, the more abundant the edge states. In Section 4.3, we specify to the Wallace model for graphene to illustrate the concepts and give numerical results on the edge states.

Finally, we provide in Appendix A a precise definition of the Spectral Flow adapted to our setting, and establish some of its properties that are used in the body of the paper.

2. SPECTRAL FLOWS IN ONE-DIMENSIONAL MODELS

In this section, we prove our results in the one-dimensional setting.

2.1. Generalities for bulk and edge Hamiltonians.

2.1.1. Bulk periodic Hamiltonians. We work in this section in the Hilbert space $\ell^2(\mathbb{Z}, \mathbb{C}^N)$, with operators that are periodic, i.e., commute with the shift operator τ_1 defined by $(\tau_1 \Psi)_n := \Psi_{n-1}$. Such operators appear in TB models for a periodic chain of atoms, and N represents the number of particles in one unit cell. The corresponding Hamiltonian can be written as a discrete convolution in the form

$$(H\Psi)_n = \sum_{m \in \mathbb{Z}} h(m) \Psi_{n-m} = (h * \Psi)_n. \quad (2)$$

Lemma 2.1. *If $h \in \ell^1(\mathbb{Z}, \mathbb{C}^{N \times N})$ and satisfies the symmetry condition $h(n)^* = h(-n)$, then H is a bounded self-adjoint operator on $\ell^2(\mathbb{Z}, \mathbb{C}^N)$.*

Proof. The symmetry condition $h(n)^* = h(-n)$ ensures that H is a symmetric operator. In addition, the fact that h is summable implies that H is a bounded operator. Indeed, by the discrete Young inequality for convolutions, we have

$$\forall \Psi \in \ell^2(\mathbb{Z}, \mathbb{C}^N), \quad \|H\Psi\|_{\ell^2} = \|h * \Psi\|_{\ell^2} \leq \|h\|_{\ell^1} \|\Psi\|_{\ell^2}, \quad \text{with} \quad \|h\|_{\ell^1} := \sum_{n=-\infty}^{\infty} \|h(n)\|_{\text{op}}.$$

So H is a bounded symmetric operator, hence self-adjoint. \square

Remark 2.2. *Throughout this section, we will use the term periodic to refer to 1-periodic models. If a Hamiltonian is periodic with period K for some integer $K > 1$, we can identify $\ell^2(\mathbb{Z}, \mathbb{C}^N)$ with $\ell^2(K\mathbb{Z}, \mathbb{C}^{KN})$ hence with $\ell^2(\mathbb{Z}, \mathbb{C}^{KN})$, and obtain a 1-periodic model with larger blocks. See Subsection 2.4 for an example of this.*

We define the unitary Fourier transform by $\mathcal{F} : \ell^2(\mathbb{Z}, \mathbb{C}^N) \rightarrow L^2([-\pi, \pi], \mathbb{C}^N)$ by

$$(\mathcal{F}[\Psi])(k) := \frac{1}{\sqrt{2\pi}} \sum_{m \in \mathbb{Z}} \Psi_m e^{-ikm}, \quad \text{so that} \quad \Psi_n = \frac{1}{\sqrt{2\pi}} \int_{-\pi}^{\pi} \mathcal{F}[\Psi](k) e^{ikn} dk, \quad (3)$$

and note that for any $u \in L^2([-\pi, \pi])$,

$$(\mathcal{F}H\mathcal{F}^*u)(k) = H_k u(k), \quad \text{with} \quad H_k := \sum_{m \in \mathbb{Z}} h(m) e^{-ikm}. \quad (4)$$

Since $h(n) = h^*(-n)$, the matrix H_k is Hermitian for all $k \in \mathbb{R}$. Let $\lambda_{1,k} \leq \dots \leq \lambda_{N,k}$ be the eigenvalues of H_k ranked in increasing order. Since the map $k \mapsto H_k$ is 2π -periodic and analytic, the maps $k \mapsto \lambda_{j,k}$ are 2π -periodic and continuous (we loose analyticity when eigenvalues intersect). In what follows, we set $\Omega^* := (-\pi, \pi]$. The spectral theorem then shows that

$$\sigma_{\text{bulk}} := \sigma(H) = \bigcup_{k \in \Omega^*} \sigma(H_k) = \bigcup_{j=1}^N \bigcup_{k \in \Omega^*} \{\lambda_{j,k}\}. \quad (5)$$

The spectrum of H consists of N *Bloch bands*, which are the images of $k \mapsto \lambda_{j,k}$. Each Bloch band is a closed interval by continuity and periodicity of this map. The intervals in the complement of this spectrum are called *gaps*, or *bulk gaps*.

2.1.2. Soft wall operators. Our goal is to study such periodic Hamiltonians, in the presence of a soft wall. Let us precise the class of walls that we use in this article.

Definition 2.3. *An operator W acting on $\ell^2(\mathbb{Z}, \mathbb{C}^N)$ is a soft wall operator if it is of the form*

$$\forall n \in \mathbb{Z}, \quad (W\Psi)_n = w(n) \Psi_n,$$

where $w : \mathbb{R} \mapsto \mathcal{S}_N$ is ν -Lipschitz for some $\nu > 0$, and satisfies (1), i.e. has the limits

$$\forall v \in \mathbb{C}^N \setminus \{0\}, \quad \lim_{x \rightarrow -\infty} \langle v, w(x)v \rangle = +\infty \quad \text{and} \quad \lim_{x \rightarrow +\infty} \langle v, w(x)v \rangle = 0.$$

The first limit implies that for all $\Sigma \in \mathbb{R}$, there is $x_\Sigma \in \mathbb{R}$ so that

$$\forall x \leq x_\Sigma, \quad w(x) \geq \Sigma.$$

Since w is Lipschitz, it is continuous. Also, since it goes from $+\infty$ to 0, it is bounded from below. The shifted, or translated, soft wall operator is

$$(W(t)\Psi)_n := w(n-t)\Psi_n.$$

It is an unbounded self-adjoint operator, with domain

$$\mathcal{D}(W(t)) := \{\Psi \in \ell^2(\mathbb{Z}, \mathbb{C}^N), \quad W(t)\Psi \in \ell^2(\mathbb{Z}, \mathbb{C}^N)\}.$$

Note that $\|W(t) - W(0)\|_{\text{op}} = \sup_{n \in \mathbb{Z}} \|w(n-t) - w(t)\|_{\text{op}} \leq \nu|t|$, so this domain is independent of t and we will denote it simply by $\mathcal{D}(W)$. Let $\mu_{1,x} \leq \dots \leq \mu_{N,x}$ be the eigenvalues of $w(x)$ for all $x \in \mathbb{R}$. Since w is ν -Lipschitz, all the curves $x \mapsto \mu_{j,x}$ are ν -Lipschitz as well. In addition, all these curves go from $+\infty$ to 0 on \mathbb{R} . As $W(t)$ is block diagonal with block elements $w(n-t)$, we directly deduce that

$$\sigma(W(t)) = \bigcup_{n \in \mathbb{Z}} \sigma(w(n-t)) = \bigcup_{j=1}^N \bigcup_{n \in \mathbb{Z}} \{\mu_{j,n-t}\}, \quad \text{and that} \quad \sigma_{\text{ess}}(W_t) = \{0\}. \quad (6)$$

The spectrum is purely discrete, composed of eigenvalues. They are all of finite multiplicities (except maybe 0), and the only accumulation point is 0. In addition, the map $t \mapsto W(t)$ is 1-quasi-periodic, in the sense that

$$W(t+1) = \tau_1^* W(t) \tau_1, \quad \text{with} \quad (\tau_1 \Psi)_n := \Psi_{n-1}.$$

In particular, the spectrum is 1-periodic (which can be read directly from (6)). See also Fig. 1 for an illustration.

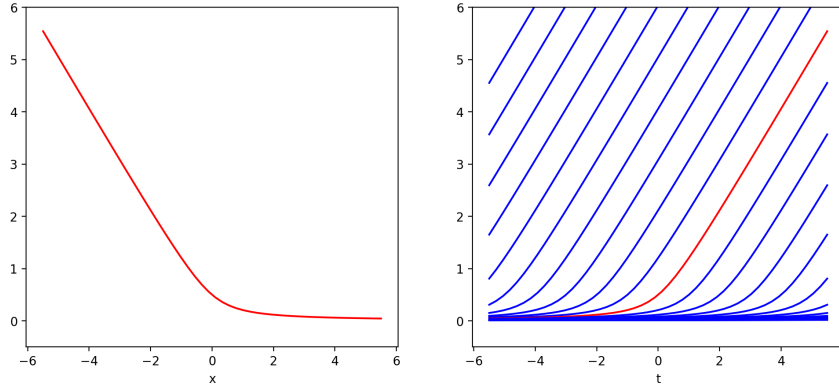


FIGURE 1. Left: the function $w(x) := \frac{1}{2}(\sqrt{x^2 + 1} - x)$, with $N = 1$. Right: the spectrum of the corresponding operator $W(t)$, as a function of t (the $n = 0$ case is in red). As t increases, the wall moves to the right. Here, $t \mapsto W(t)$ is operator increasing.

We define the *edge* operator $H^\sharp(t) := H + W(t)$. Let us record some properties for this operator.

Proposition 2.4. *Let $w : \mathbb{R} \mapsto \mathcal{S}_N$ be a Lipschitz function satisfying (1).*

- (1) *For all $t \in \mathbb{R}$, the operator $H^\sharp(t)$ is self-adjoint on the constant domain $\mathcal{D}(W)$.*
- (2) *The map $t \mapsto H^\sharp(t)$ is norm-resolvent continuous and 1-quasi-periodic, in the sense that $H^\sharp(t+1) = \tau_1^* H^\sharp(t) \tau_1$, where τ_1 is the usual translation operator $(\tau_1 \Psi)_n := \Psi_{n-1}$;*
- (3) *The essential spectrum $\sigma_{\text{ess}}(H^\sharp(t))$ is independent of t , and equals σ_{bulk} .*

Proof of Proposition 2.4. For the first point, the bulk operator H is bounded and self-adjoint, hence is a bounded perturbation of the self-adjoint operator $W(t)$. Thus, $H^\sharp(t)$ is self-adjoint on $\mathcal{D}(W)$.

For the second point, note that H is independent of t while the map $t \mapsto W(t)$ is norm-resolvent continuous. Indeed, the operator $(i - W(t))^{-1}$ is block diagonal with block elements $(i - w(n - t))^{-1}$, and we have the bound

$$\begin{aligned} \left\| \frac{1}{i - w(n - t)} - \frac{1}{i - w(n - t')} \right\|_{\text{op}} &= \left\| \frac{1}{i - w(n - t)} [w(n - t) - w(n - t')] \frac{1}{i - w(n - t')} \right\|_{\text{op}} \\ &\leq \nu |t' - t|. \end{aligned}$$

The quasi-periodicity follows from the quasi-periodicity of $W(t)$ and the periodicity of H . Since τ_1 is unitary, it implies that the spectrum of $H^\sharp(t)$ is 1-periodic in t .

It remains to prove the third point, and compute the essential spectrum of $H^\sharp(t)$. We omit the argument t for shortness. We identify $\ell^2(\mathbb{Z}, \mathbb{C}^N)$ with $\ell^2(\mathbb{Z}^-, \mathbb{C}^N) \oplus \ell^2(\mathbb{Z}^+, \mathbb{C}^N)$ and define the restrictions Π_L from $\ell^2(\mathbb{Z}, \mathbb{C}^N)$ onto $\ell^2(\mathbb{Z}^-, \mathbb{C}^N)$ and Π_R from $\ell^2(\mathbb{Z}, \mathbb{C}^N)$ onto $\ell^2(\mathbb{Z}^+, \mathbb{C}^N)$. We write

$$H^\sharp = H_L^\sharp \oplus H_R^\sharp + K, \quad \text{with} \quad H_L^\sharp = \Pi_L H^\sharp \Pi_L^*, \quad H_R^\sharp(t) = \Pi_R H^\sharp \Pi_R^*$$

and

$$K = \Pi_R H^\sharp \Pi_L^* + \Pi_L H^\sharp \Pi_R^* = \Pi_R H \Pi_L^* + \Pi_L H \Pi_R^*,$$

where the last equality comes from the fact that W is diagonal. First, we claim that K is a compact operator. Indeed, for $\ell \in \mathbb{N}$, we introduce the finite range one-periodic Hamiltonian

$$H_\ell \Psi := h_\ell * \Psi, \quad \text{with kernel} \quad h_\ell(n) = h(n) \mathbf{1}(|n| \leq \ell). \quad (7)$$

Since h_ℓ converges to h in $\ell^1(\mathbb{Z}, \mathbb{C}^{N \times N})$, we have $\|H - H_\ell\|_{\text{op}} \rightarrow 0$ as $\ell \rightarrow \infty$ by Young's inequality (see the proof of Lemma 2.1). So we also have $\|K - K_\ell\|_{\text{op}} \rightarrow 0$, with $K_\ell := \Pi_R H_\ell \Pi_L^* + \Pi_L H_\ell \Pi_R^*$. In addition, K_ℓ is finite rank for all $\ell > 0$, so K is compact, as stated.

Since K is compact, it does not affect the essential spectrum, so $\sigma_{\text{ess}}(H^\sharp) = \sigma_{\text{ess}}(H_L^\sharp) \cup \sigma_{\text{ess}}(H_R^\sharp)$. Let us identify the essential spectra of H_L^\sharp and H_R^\sharp . To the right of the wall, W is bounded and decays to zero. Thus, $\Pi_R W \Pi_R^*$ is compact and

$$\sigma_{\text{ess}}(H_R^\sharp) = \sigma_{\text{ess}}(H_R).$$

A convenient way to identify $\sigma_{\text{ess}}(H_R)$ is to note that, again by compactness of K ,

$$\sigma_{\text{bulk}} = \sigma_{\text{ess}}(H_L) \cup \sigma_{\text{ess}}(H_R),$$

but $\sigma_{\text{ess}}(H_L) = \sigma_{\text{ess}}(H_R)$, since a reflection around $-1/2$ maps H_L to H_R . Hence, $\sigma_{\text{ess}}(H_R^\sharp) = \sigma_{\text{bulk}}$.

To the left of the wall, W_L has compact resolvent, since it has eigenvalues of finite multiplicity and without accumulation points. Since H is bounded, $H_L(W_L - i)^{-1}$ is compact and $\sigma_{\text{ess}}(H_L^\sharp) = \sigma_{\text{ess}}(W_L) = \emptyset$. \square

2.2. Computation of the spectral flow: reduction to the Jacobi case. We now compute the spectral flow of $t \mapsto H^\sharp(t)$. Recall that, for $E \in \mathbb{R} \setminus \sigma_{\text{bulk}}$, the spectral flow $\text{Sf}(H^\sharp(t), E, [0, 1])$ counts the net number of eigenvalue branches that cross E downwards, as t varies between 0 and 1. A precise definition together with some properties can be found in Appendix A. The following example illustrates the concept.

Example 2.1. For the soft wall operator $t \mapsto W(t)$, we have

$$\forall E > 0, \quad \text{Sf}(W(t), E, [0, 1]) = -N, \quad \text{while} \quad \forall E < 0, \quad \text{Sf}(W(t), E, [0, 1]) = 0.$$

This can be seen directly from Figure 1. This case fits in the framework of Theorem 1.1 with $H = 0$, since in this case the N bands consist of the singleton 0.

We will take advantage of the robustness of the spectral flow and reduce the problem to simpler models. For instance, we will first prove the results for 1-periodic Jacobi operators (for which $h(n) = 0$ for $|n| \geq 2$), and then extend it to all 1-periodic Hamiltonians by density. The proof that the spectral flow equals $-N(E)$ for Jacobi operator is postponed to the next Section. In this section, we explain how to generalize the result for Jacobi operators to any periodic Hamiltonian.

A *Jacobi operator* is an operator H acting on $\ell^2(\mathbb{Z}, \mathbb{C}^N)$ of the form

$$\forall \Psi \in \ell^2(\mathbb{Z}, \mathbb{C}^N), \quad (H\Psi)_n := a_{n-1}^* \Psi_{n-1} + b_n \Psi_n + a_n \Psi_{n+1}, \quad (8)$$

where $(a_n)_{n \in \mathbb{Z}}$ and $(b_n)_{n \in \mathbb{Z}}$ are two families of complex-valued $N \times N$ matrices, with $b_n = b_n^*$. We will often represent such operators with a block matrix of the form

$$H = \left(\begin{array}{ccc|cc} \ddots & \ddots & & & \\ & \ddots & b_{-2} & a_{-2} & \\ & & a_{-2}^* & b_{-1} & a_{-1} \\ \hline & & & a_{-1}^* & b_0 & a_0 \\ & & & & a_0^* & b_1 & \ddots \\ & & & & & \ddots & \ddots \end{array} \right).$$

We used the canonical basis of $\ell^2(\mathbb{Z}, \mathbb{C}^N)$, and the two straight lines indicate the decomposition $\mathbb{Z} = \mathbb{Z}^- \cup \mathbb{Z}^+$ with $\mathbb{Z}^- := \{n \in \mathbb{Z}, n < 0\}$ and $\mathbb{Z}^+ = \{n \in \mathbb{Z}, n \geq 0\}$. A Jacobi operator is K -periodic if $a_{n+K} = a_n$ and $b_{n+K} = b_n$. It is 1-periodic, or simply periodic, if $b_n = b$ and $a_n = a$ are independent of $n \in \mathbb{Z}$. Periodic Jacobi operators are of the convolution form (2) with

$$h(-1) = a, \quad h(0) = b, \quad h(1) = a^*.$$

In this simple case, the bulk spectrum (5) is given by

$$\sigma_{\text{bulk}} := \sigma(H) = \bigcup_{k \in \Omega^*} \sigma(H_k) \quad \text{with} \quad H_k := a^* e^{-ik} + b + a e^{ik}. \quad (9)$$

We will establish a version of Theorem 1.1 in the special of Jacobi operators.

Proposition 2.5. *Let H be a Jacobi operator and $w : \mathbb{R} \mapsto \mathcal{S}_N$ be a Lipschitz function satisfying (1). Define the operator family $H^\sharp(t)$ as in Section 2.1.2. For all $E \in \mathbb{R} \setminus \sigma_{\text{bulk}}$, the energy E is in the essential gaps of all operators $H^\sharp(t)$, and*

$$\text{Sf}(H^\sharp(t), E, [0, 1]) = -\mathcal{N}(E).$$

The proof of this Proposition is technically the most involved part of the paper. Its full proof is the topic of Section 3. For now, let us explain how to deduce Theorem 1.1 from it, that is how to go from the periodic Jacobi case to the general 1-periodic Hamiltonians.

Proof of Theorem 1.1 as a corollary of Proposition 2.5. First, we explain how the case of finite-range interactions can be reduced to the Jacobi case, using *supercells*, and next we show that convolution by ℓ^1 -kernels can be approximated by finite rank kernels.

Step 1 : From 1-periodic Jacobi operators to finite range interactions. Assume indeed that the periodic Hamiltonian H has a kernel h with finite range, say $h(n) = 0$ for all $n > \ell$. Then we can write H as a Jacobi operator acting on $\ell^2(\ell\mathbb{Z}, \mathbb{C}^{\ell N})$, by defining the supercell kernel \tilde{h} with

$$\tilde{h}(-1) = \tilde{a}, \quad \tilde{h}(0) = \tilde{b}, \quad \tilde{h}(1) = \tilde{a}^*.$$

where \tilde{b} and \tilde{a} are matrices of size $(\ell N) \times (\ell N)$, given by

$$\tilde{b} := \begin{pmatrix} h(0) & h(-1) & \cdots & h(-\ell+1) \\ h(1) & h(0) & \cdots & h(-\ell+2) \\ \vdots & \ddots & \ddots & \vdots \\ h(\ell-1) & \cdots & h(1) & h(0) \end{pmatrix} \quad \text{and} \quad \tilde{a} := \begin{pmatrix} h(-\ell) & 0 & \cdots & 0 \\ h(-\ell+1) & h(-\ell) & \ddots & \vdots \\ \vdots & \vdots & \ddots & 0 \\ h(-1) & h(-2) & \cdots & h(-\ell) \end{pmatrix}.$$

If \tilde{H} denotes the corresponding operator on $\ell^2(\mathbb{Z}, \mathbb{C}^{\ell N})$, then $\sigma(H) = \sigma(\tilde{H})$, and each Bloch band of H becomes a set of ℓ bands for \tilde{H} . In particular, $\mathcal{N}_{\tilde{H}}(E) = \ell \mathcal{N}_H(E)$.

For the supercell soft wall, we set

$$\tilde{w}(x) := \begin{pmatrix} w(\ell x) & 0 & \cdots & 0 \\ 0 & w(\ell x + 1) & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & w(\ell x + \ell - 1) \end{pmatrix}$$

and define $\tilde{W}(t)$ by the construction in Subsection 2.1.2. The operator $\tilde{H}^\sharp(t) := \tilde{H} + \tilde{W}(t)$ is a periodic Jacobi operator with the same spectrum as the original $H^\sharp(\ell t)$. As t increases from 0 to 1, the parameter ℓt varies from 0 to ℓ . In particular, the spectral flow satisfies

$$\text{Sf} \left(\tilde{H}^\sharp(t), [0, 1], E \right) = \text{Sf} \left(H^\sharp(t), [0, \ell], E \right) = \ell \text{Sf} \left(H^\sharp(t), [0, 1], E \right).$$

On the other hand, Proposition 2.5 gives

$$\text{Sf} \left(\tilde{H}^\sharp(t), [0, 1], E \right) = -\mathcal{N}_{\tilde{H}}(E) = -\ell \mathcal{N}_H(E),$$

which proves Theorem 1.1 in the case of finite range kernels.

Step 2 : From finite range to integrable kernels. Now consider a general kernel h in ℓ^1 . For $\ell \in \mathbb{N}$, we consider the periodic Hamiltonian H_ℓ with finite range potential

$$h_\ell(n) := h(n) \mathbf{1}(|n| \leq \ell).$$

This kernel has already been introduced in (7). Recall that $\|H - H_\ell\|_{\text{op}} \rightarrow 0$ by Young's inequality. Note also that $\|H^\sharp(t) - H_\ell^\sharp(t)\|_{\text{op}} = \|H - H_\ell\|_{\text{op}}$ is independent of t , hence goes to 0 uniformly in $t \in \mathbb{R}$. In particular, the spectrum of $H_\ell^\sharp(t)$ approaches uniformly the spectrum of $H^\sharp(t)$.

Let us fix $E \in \mathbb{R} \setminus \sigma_{\text{bulk}}$ and set

$$\varepsilon := \text{dist}(E, \sigma_{\text{bulk}}) > 0.$$

The previous point shows that there exists ℓ_0 such that, for all $\ell \geq \ell_0$, we have $\|H - H_\ell\|_{\text{op}} \leq \varepsilon/2$. For $\ell \geq \ell_0$, we obtain that E is not the essential spectrum of $H_\ell^\sharp(t)$ for all t , hence the spectral flow $\text{Sf} \left(H_\ell^\sharp(t), [0, 1], E \right)$ is well-defined. In addition, we have, with obvious notations, $\mathcal{N}_{H_\ell}(E) = \mathcal{N}_H(E)$ for $\ell \geq \ell_0$.

We can now apply the robustness of the spectral flow with respect to small bounded perturbation, see Lemma A.9 in the Appendix, and get that

$$\text{Sf} \left(H^\sharp(t), [0, 1], E \right) = \lim_{\ell \rightarrow \infty} \text{Sf} \left(H_\ell^\sharp(t), [0, 1], E \right) = -\mathcal{N}(E),$$

where we used that Theorem 1.1 holds for finite range interactions. \square

2.3. The spectrum at fixed t_0 , proof of Theorem 1.3. In this section, we prove Theorem 1.1, which states that for all t_0 and all $E \in \mathbb{R} \setminus \sigma_{\text{bulk}}$, there are at least $\mathcal{N}(E)$ eigenvalues in each interval of size ν in the gap where E lies.

Proof. The main argument is that since $t \mapsto H^\sharp(t)$ is ν -Lipschitz, so are all the eigenvalues branches. Let $E \in \mathbb{R} \setminus \sigma_{\text{bulk}}$ with $\mathcal{N}(E) > 0$. Since there is a nonzero spectral flow, $H^\sharp(t)$ has eigenvalues for at least some values of t . By shifting t if necessary, we may assume $t = 0$. We label this eigenvalue $\lambda_0(0)$ and use this as a starting point to label the eigenvalue curves $\lambda_k(t)$ for $t \in [0, 1]$ such that, for all $t \in [0, 1]$

$$\lambda_k(t) \leq \lambda_{k+1}(t), \text{ where } k \in \mathbb{Z},$$

and with the convention that $\lambda_k(t)$ equals the edge of the essential spectrum if there exists no k -th eigenvalue at this value of t . Since the spectrum is periodic, we have $\lambda_k(1) = \lambda_j(0)$ for some $j \in \mathbb{Z}$. The spectral flow equals $-\mathcal{N}(E)$, so there are exactly $\mathcal{N}(E)$ eigenvalues that crosses $\lambda_k(1)$

upwards. We deduce that we actually have $\lambda_k(1) = \lambda_{k+\mathcal{N}(E)}(0)$ for all values of $k \in \mathbb{Z}$ such that $\lambda_k(0)$ is an eigenvalue of $H^\sharp(0)$. Then, the Lipschitz continuity of $t \mapsto \lambda_k(t)$ gives

$$\lambda_{k+\mathcal{N}(E)}(0) - \lambda_k(0) = \lambda_k(1) - \lambda_k(0) \leq \nu.$$

Hence, there are at least $\mathcal{N}(E)$ eigenvalues for $H^\sharp(0)$ in each interval of length ν in the gap. If ν is larger than the width of the gap, the same argument shows that there is edge spectrum for any $t_0 \in [0, 1]$, and we can repeat the counting argument for this t_0 . \square

2.4. Example : the SSH model. Before going to the technicalities of the proof, let us illustrate our Theorem in the case of the Su–Schrieffer–Heeger (SSH) model [30].

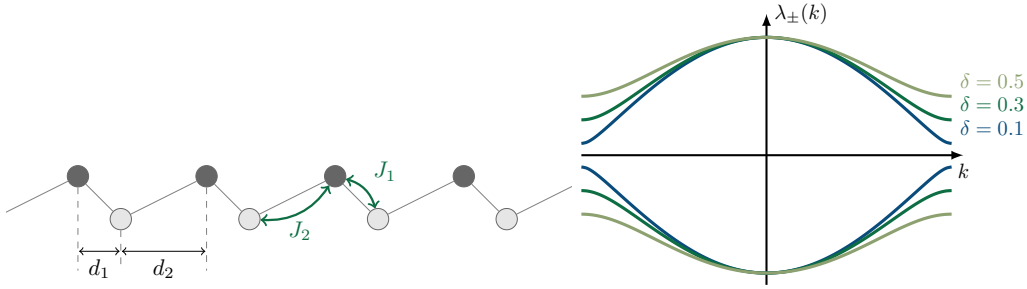


FIGURE 2. Left: illustration of the SSH model. Right: its band structure for different values of $\delta := ||J_1| - |J_2||$.

2.4.1. Presentation of the model, and basic facts. The SSH model is a tight-binding Hamiltonian describing a polyacetylene chain, a simple polymer where the distance between neighboring carbon-hydrogen (CH) pairs takes alternating values. We denote by $d_1 > 0$ (resp. $J_1 \in \mathbb{C}$) the distance (resp. hopping amplitude) between the $(2n)$ -th (CH) pair and the $(2n+1)$ -th one, and by $d_2 = 1 - d_1 > 0$ (resp. $J_2 \in \mathbb{C}$) the ones between $(2n+1)$ -th and the $(2n+2)$ -th. If $d_1 \neq d_2$, then the distances alternate, hence so are the hopping parameters, see Figure 2. In the tight-binding approximation (and for an idealized infinite chain), the Hamiltonian takes the form of a 2-periodic Jacobi operator acting on $\ell^2(\mathbb{Z}, \mathbb{C})$ with alternating hopping strengths J_1 and J_2 , that is

$$\begin{pmatrix} \ddots & \ddots & & & & \\ & \ddots & 0 & J_1 & & \\ & & J_1^* & 0 & J_2 & \\ & & & J_2^* & 0 & J_1 \\ & & & & J_1^* & 0 & \ddots \\ & & & & & \ddots & \ddots \end{pmatrix}.$$

In most cases, we take J_1, J_2 real numbers. Complex values of J_1, J_2 happen to appear in the case of the Wallace model for graphene with zigzag cuts. In this case, the phases can be removed by defining a *gauge transformation* $U = e^{iA}$ where A is the multiplication operator by

$$A_n = \begin{cases} \sum_{j=0}^{n-1} \phi_j & n \geq 1 \\ 0 & n = 0 \\ -\sum_{j=n}^{-1} \phi_j & n \leq -1 \end{cases} \quad \text{with } \phi_n = \begin{cases} \arg J_1 & n \text{ odd} \\ \arg J_2 & n \text{ even} \end{cases}.$$

The SSH Hamiltonian becomes a 1-periodic Jacobi operator H if we take $N = 2$ and the 2×2 blocks

$$b = \begin{pmatrix} 0 & J_1 \\ J_1^* & 0 \end{pmatrix} \quad \text{and} \quad a = \begin{pmatrix} 0 & 0 \\ J_2 & 0 \end{pmatrix}. \quad (10)$$

According to (9), the bulk spectrum can be computed from

$$H_k = b + ae^{ik} + a^*e^{-ik} = \begin{pmatrix} 0 & J_1 + J_2e^{-ik} \\ J_1 + J_2e^{ik} & 0 \end{pmatrix},$$

whose spectrum is $\pm|J_1 + J_2e^{ik}|$. Note that, as k varies on \mathbb{R} , the complex number $J_1 + J_2e^{ik}$ describes a circle with center J_1 , and radius $|J_2|$. With this in mind, we conclude that

$$\sigma_{\text{bulk}} := \sigma(H) = \sigma_{\text{ess}}(H) = [-W, -\delta] \cup [\delta, W], \quad W := |J_1| + |J_2|, \quad \delta := ||J_1| - |J_2||.$$

In particular, if $|J_1| \neq |J_2|$, there is a gap of size $2\delta > 0$ around the origin, separating the two Bloch bands. In this gap, we have $\mathcal{N}(E) = 1$.

Remark 2.6 (Hard truncation for SSH). *For the hard cut Hamiltonian*

$$H^\sharp := \begin{pmatrix} 0 & J_1 & & \\ J_1^* & 0 & J_2 & \\ & J_2^* & 0 & \ddots \\ & & \ddots & \ddots \end{pmatrix},$$

seen as an operator on $\ell^2(\mathbb{N}_0, \mathbb{C})$ (without supercell), then any $\psi \in \ell^2(\mathbb{N}_0, \mathbb{C})$ solution to $H^\sharp \psi = 0$ solves $J_1\psi_1 = 0$ and $\psi_{n+2} = \frac{-J_1^*}{J_2}\psi_n$ for all $n \geq 0$. We easily deduce that $\psi_{2n+1} = 0$, and that ψ is non null and square integrable at $+\infty$ iff $|J_1| < |J_2|$. So $0 \in \sigma(H^\sharp)$ iff $|J_1| < |J_2|$. When the hard cut is translated, and crosses one atom, the role of J_1 and J_2 are exchanged. So, depending on the location of the hard cut, the eigenvalue 0 is a (protected) eigenvalue, or is not an eigenvalue.

2.4.2. Numerical simulations for the SSH chain. We now compute numerically the spectral flow in the SSH model, in the presence of a shifted soft wall. For the soft wall, we take

$$w(x) = \begin{pmatrix} w_1(x) & 0 \\ 0 & w_1(x + d_1) \end{pmatrix} \quad \text{with} \quad w_1(x) := \begin{cases} 0 & \text{for } x \geq 0 \\ -\nu x & \text{for } x \leq 0 \end{cases},$$

which corresponds to the evaluation of w_1 at the location of each of the two atoms in the first unit cell. Note that w satisfy the assumption of a soft-wall, and is ν -Lipschitz.

To compute the edge spectrum of the edge operator, we choose the following simple procedure: we restrict $H^\sharp(t)$ to the box $[-L, L]$ (with $2L + 1$ unit cells), so we consider the finite matrices

$$H_L^\sharp(t) := \begin{pmatrix} b & a & & \\ a^* & b & a & \\ 0 & \ddots & \ddots & \ddots \\ & & a^* & b & a \\ & & & a^* & b \end{pmatrix} + \begin{pmatrix} W_t(-L) & & & \\ & W_t(-L+1) & & \\ & & \ddots & \\ & & & W_t(L) \end{pmatrix}.$$

Then, for each eigenpair (λ, u) with $\|u\|_{\ell_L^2} = 1$, we check if the mass of u is localized near the origin, or, more specifically, not localized at the boundary of our simulation box. This procedure discards the spurious edge modes due to the truncation. We detect that u is an *true* edge mode whenever $\|u\mathbf{1}(-L/2 \leq n \leq L/2)\|_{\ell_L^2} \geq 3/4$.

For our numerical simulations, we took $d_1 = 1/4$ (so $d_2 = 3/4$) for the distances between the atoms, $J_1 = 3/2$ and $J_2 = 1/2$ for the hopping parameters, $L = 100$, and we took different values of $\nu \in [0.5, 1, 5, 10]$. The results are displayed in Figure 3. In each of these figures, we observe a spectral flow of -1 in the middle gap, and of -2 above the second Bloch band, in accordance with Theorem 1.1. The flow of eigenvalues becomes steeper and steeper as ν increases, as predicted in Theorem 1.3. Note that our soft wall w is continuous, but not continuously differentiable. This explains the *kinks* in the Right figures ($\nu = 5$ and $\nu = 10$), which happens when the kink of the wall touches the second atom located at $x_2 = 1/4$. Note also that since we took $x \mapsto w_1$ non-increasing, the maps $t \mapsto W(t)$ and $t \mapsto H^\sharp(t)$ are operator non-decreasing. So all eigenvalue branches are non-decreasing, as can be checked on these pictures.

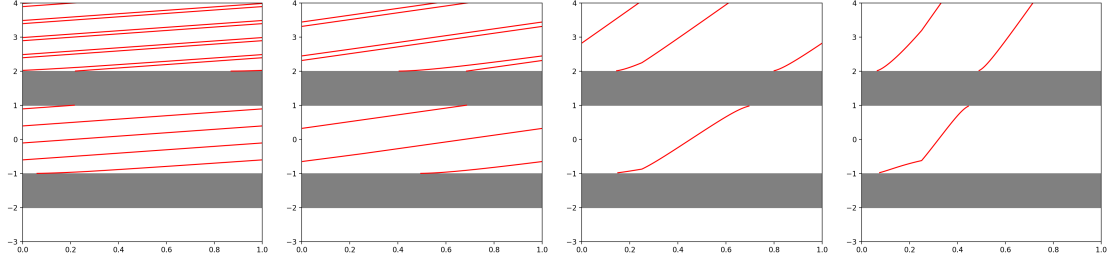


FIGURE 3. Numerics for the spectrum of $t \mapsto H^\sharp(t)$ in the SSH model, for different values of ν . From left to right, $\nu = 0.5$, $\nu = 1$, $\nu = 5$ and $\nu = 10$. The essential spectrum is displayed in grey, and the edge spectrum in red. For E in the gap between the 2 bands, $\mathcal{N}(E) = 1$ and the spectral flow is -1 , above the bands, $\mathcal{N}(E) = 2$ and the spectral flow equals -2 .

Finally, the first two simulations correspond to values of ν smaller than the size of the gap ($2|J_1 - J_2| = 2$) and we can observe that the lower bound on the number of eigenvalues from Theorem 4.2 is almost achieved here.

3. COMPUTATION OF SPECTRAL FLOWS IN THE JACOBI CASE

It remains to prove Proposition 2.5, that is to prove that the spectral flow is $-\mathcal{N}(E)$ in the case of periodic Jacobi operators. In order to do so, we will use the robustness of the spectral flow to make successive modifications to the operators. In Subsections 3.1, the Jacobi operator $H^\sharp(t)$ will be shown to have the same spectral flow as a *cut* model $H_{\text{cut}}^\Sigma(t)$, which, itself, has a same spectral flow equal to a dislocated model $\tilde{H}(t)$, see Subsection 3.2. This last spectral flow can be computed explicitly, and turns out to be equal to $-\mathcal{N}(E)$.

Before we start, we emphasize that several techniques are available to study Jacobi operators, such as the ones involving *transfer matrices*. Recall indeed that if H is Jacobi, then the equation $H\Psi = E\Psi$ implies that

$$\begin{pmatrix} \Psi_{n+1} \\ \Psi_n \end{pmatrix} = T(E) \begin{pmatrix} \Psi_n \\ \Psi_{n-1} \end{pmatrix}, \quad \text{with} \quad T(E) := \begin{pmatrix} -a^{-1}(b - E) & -a^{-1}a^* \\ 1 & 0 \end{pmatrix},$$

so that we can study the properties of Ψ by studying the transfer matrix $T(E)$. However, this matrix is not always well-defined (in the previous formulation, we need a to be invertible for instance). Actually, we were not able to recover our results using the formalism of transfer matrices. Our proof rather relies on a direct study of the full operator, and a variational argument.

3.1. Reduction to the cut case. We first deform the potential w to a simpler form. In what follows, we fix a Jacobi operator $H \in \ell^2(\mathbb{Z}, \mathbb{C}^N)$ with kernel h having diagonal entries b and off-diagonal entries a . Let us fix $E \in \mathbb{R} \setminus \sigma_{\text{bulk}}$, and consider some $\Sigma \in \mathbb{R}$ large enough so that

$$\Sigma \geq E + 4C_{a,b} + 1, \quad \text{with} \quad C_{a,b} := \max\{\|a\|_{\text{op}}, \|b\|_{\text{op}}\}.$$

Since $w(x) \rightarrow +\infty$ as $x \rightarrow -\infty$, there is $x_\Sigma \in \mathbb{R}$ so that $w(x) \geq \Sigma$ for all $x < x_\Sigma$. Without loss of generality, we may assume $x_\Sigma \leq -1$. We consider the modified potential (here and in what follows, Σ is shorthand for $\Sigma \mathbb{I}_N$)

$$w_\Sigma(x) := \begin{cases} 0 & \text{if } x \geq 0, \\ -x(\Sigma - b) & \text{if } x \in [-1, 0], \\ (\Sigma - b) & \text{if } x \in [x_\Sigma, -1], \\ (x - x_\Sigma + 1)(\Sigma - b) + (x_\Sigma - x)w(x) & \text{if } x \in [x_\Sigma - 1, x_\Sigma], \\ w(x) & \text{if } x \leq x_\Sigma - 1. \end{cases} \quad (11)$$

We also denote by $W_\Sigma(t)$ the corresponding modified wall operator. The key properties of w_Σ and W_Σ are summarized in the following straightforward Lemma.

Lemma 3.1. *The potential w_Σ is Lipschitz (hence continuous), is linear on $[-1, 0]$ and satisfies*

$$\forall x > 0, \quad w_\Sigma(x) = 0, \quad \text{while} \quad \forall x < -1, \quad w_\Sigma(x) \geq E + 3C_{a,b} + 1.$$

Proof. The first points are obvious. If $x < -1$, we note that $(\Sigma - b) \geq \Sigma - \|b\|_{\text{op}} \geq E + 3C_{a,b} + 1$ and that, if $x < x_\Sigma \leq -1$, we also have $w(x) \geq \Sigma \geq E + 3C_{a,b} + 1$. The last inequality follows since w_Σ is a combination of these two matrices for $x < -1$. \square

The difference of potentials $w - w_\Sigma$ is continuous, vanishes for $x < x_\Sigma$, and goes to 0 as $x \rightarrow +\infty$. In particular, for all $t \in \mathbb{R}$, $(W - W_\Sigma)(t)$ is compact, and the map $t \mapsto (W - W_\Sigma)(t)$ is continuous and 1-quasi-periodic.

Let $H^\Sigma(t) := H + W_\Sigma(t)$ be the corresponding edge Hamiltonian. We have

$$H^\Sigma(t) - H^\sharp(t) = W(t) - W_\Sigma(t),$$

which is compact for all $t \in \mathbb{R}$. In addition, both operators H^Σ and H^\sharp are 1-quasi-periodic. By robustness of the spectral flow with respect to compact operators, see Lemma A.11, we deduce that

$$\text{Sf}(H^\sharp(t), E, [0, 1]) = \text{Sf}(H^\Sigma(t), E, [0, 1]). \quad (12)$$

In what follows, we study the operator $H^\Sigma(t)$. The main advantage of this new potential w_Σ is that it is piece-wise linear for $x \in [-1, 0]$.

Our goal is now to compute the spectral flow of $t \mapsto H^\Sigma(t)$. For $t \in [0, 1]$ we define the cut operator

$$K(t) := \left(\begin{array}{ccc|cc} \ddots & & \ddots & & \\ \ddots & & 0 & (1-t)a & \\ & (1-t)a^* & 0 & & \\ & & a^* & & \\ \hline & & & a & \\ & & & 0 & ta \\ & & & ta^* & 0 & \ddots \\ & & & & \ddots & \ddots \end{array} \right),$$

where all undisplayed matrix elements are 0. This operator is piece-wise linear, of the form $K(t) = tK(1) + (1-t)K(0)$, with

$$K(0) = \left(\begin{array}{ccc|cc} \ddots & & \ddots & & \\ \ddots & & 0 & a & \\ & a^* & 0 & & \\ & & a^* & & \\ \hline & & & a & \\ & & & 0 & 0 \\ & & & 0 & 0 & \ddots \\ & & & & \ddots & \ddots \end{array} \right), \quad K(1) = \left(\begin{array}{ccc|cc} \ddots & & \ddots & & \\ \ddots & & 0 & 0 & \\ & 0 & 0 & a & \\ & & a^* & 0 & a \\ \hline & & & a^* & 0 & \ddots \\ & & & & \ddots & \ddots \end{array} \right).$$

Note that $K(1) = \tau_1 K(0) \tau_1^*$, so the map $t \mapsto K(t)$ can be extended by 1-quasi-periodicity, and this extension is continuous. For simplicity, in what follows, we will restrict the study to $t \in [0, 1]$.

We now define the cut Jacobi operator

$$H_{\text{cut}}^\Sigma(t) := H^\Sigma(t) - K(t), \quad \text{so that} \quad H^\Sigma(t) = H_{\text{cut}}^\Sigma(t) + K(t)$$

Since $t \mapsto H^\Sigma(t)$ and $t \mapsto K(t)$ are continuous and 1-quasi-periodic, so is $t \mapsto H_{\text{cut}}^\Sigma(t)$. So, using again the robustness of the spectral flow with respect to compact, quasi-periodic operators, see Lemma A.11, we find that

$$\text{Sf}(H^\Sigma(t), E, [0, 1]) = \text{Sf}(H_{\text{cut}}^\Sigma(t), E, [0, 1]).$$

Also, by construction of the cut operator, for all $t \in [0, 1]$, $H_{\text{cut}}^\Sigma(t)$ is block diagonal with respect to the decomposition $\mathbb{Z} = \mathbb{Z}^- \cup \mathbb{Z}^+$ (note that this is no longer the case for $t \in \mathbb{R} \setminus [0, 1]$). We write $H_{\text{cut}}^\Sigma(t) = H_L^\Sigma(t) \oplus H_R^\Sigma(t)$. In an analogous way, we decompose the bulk operator as $H_{\text{cut}}(t) =$

$H_L(t) \oplus H_R(t)$ and the wall operator as $W(t) = W_L(t) \oplus W_R(t)$, so that $H_L^\Sigma(t) = H_L(t) + W_L(t)$ and $H_R^\Sigma(t) = H_R(t) + W_R(t)$.

These left and right maps are not periodic nor 1-quasi-periodic in t . Still, one can define the spectral flow as the net number of eigenvalues crossing the energy E downwards. Since these operators are no longer 1-quasi-periodic, a priori this spectral flow could depend on the value of E in the essential gap (see Appendix A). In any case, since $H_{\text{cut}}^\Sigma(t)$ is block diagonal, we have

$$\text{Sf}(H_{\text{cut}}^\Sigma(t), E, [0, 1]) = \text{Sf}(H_L^\Sigma(t), E, [0, 1]) + \text{Sf}(H_R^\Sigma(t), E, [0, 1]).$$

Lemma 3.2. *We have $\text{Sf}(H_L^\Sigma(t), E, [0, 1]) = 0$ and thus*

$$\text{Sf}(H^\Sigma(t), E, [0, 1]) = \text{Sf}(H_R^\Sigma(t), E, [0, 1]).$$

Proof. We write $H_L^\Sigma(t) = H_L(t) + W_L(t)$. Explicitly, the matrix representing $H_L(t)$ is given by (we keep the straight lines to emphasize that this matrix is only infinite in one direction)

$$H_L(t) = \begin{pmatrix} \ddots & & \ddots & & \\ & \ddots & & & \\ & & b & a & \\ & & a^* & b & ta \\ & & & ta^* & b \end{pmatrix}.$$

Note that $H_L(t)$ is a bounded operator on $\ell^2(\mathbb{Z}^-, \mathbb{C}^N)$, with uniform bound

$$\forall t \in [0, 1], \quad \|H_L(t)\|_{\text{op}} \leq 3C_{a,b}.$$

Indeed, we have, using that $0 \leq t \leq 1$, and with $\Psi_0 := 0$, that

$$\|H_L(t)\Psi\|_{\ell^2}^2 \leq \sum_{n=-\infty}^{-1} (\|a^*\|_{\text{op}}\|\Psi_{n-1}\| + \|b\|_{\text{op}}\|\Psi_n\| + \|a\|_{\text{op}}\|\Psi_{n+1}\|)^2 \leq C_{a,b}3 \sum_{n=-\infty}^{-1} \|\Psi_n\|^2 = 3C_{a,b}\|\Psi\|_{\ell^2}^2.$$

On the other hand, $W_L(t)$ is block diagonal with block elements involving $w_\Sigma(n-t)$. Since $n \leq -1$ and $t \in [0, 1]$, we have $n-t \leq -1$, so $W_L(t) \geq \Sigma - \|b\|_{\text{op}}$. Hence,

$$H_L^\Sigma(t) \geq W_L(t) - \|H_L(t)\|_{\text{op}} \geq \Sigma - \|b\|_{\text{op}} - 3C_{a,b} \geq E + 1,$$

by our choice of Σ in (11). As a consequence, E is never in the spectrum of $H_L^\Sigma(t)$. This proves the lemma. \square

We now focus on the right part. Due to our specific piece-wise linear choices for w_Σ and for the cut operator $K(t)$, we obtain that $H_R^\Sigma(t)$ is also piece-wise linear, of the form $H_R^\Sigma(t) = (1-t)H_R^\Sigma(0) + tH_R^\Sigma(1)$, with

$$H_R^\Sigma(0) = \begin{pmatrix} b & a & & \\ a & b & a & \\ & a & b & \ddots \\ & & \ddots & \ddots \end{pmatrix}, \quad \text{and} \quad H_R^\Sigma(1) = \begin{pmatrix} \Sigma & 0 & & \\ 0 & b & a & \\ & a & b & \ddots \\ & & \ddots & \ddots \end{pmatrix}.$$

As noted before, the half-line operators are no longer 1-quasi-periodic: the presence of the boundary at 0 makes the model at $t = 1$ not unitarily equivalent to the one at $t = 0$. The key observation is that the relevant part of the spectrum is still periodic, since $H_R^\Sigma(1)$ is a direct sum of Σ with (a shifted version of) $H_R^\Sigma(0)$. We will study such families of operators in the next section.

3.2. Dislocated Jacobi operators. In order to study the right-half Jacobi operator $H_R^\Sigma(t)$, we study yet another *dislocated* model. The idea to study this model comes from Hempel and Kohlmann in [21, 22], and was used in [16, 18] to compute some spectral flows for continuous Schrödinger operators acting on a one-dimensional channel. In this setting, the dislocated model is modelled by a Schrödinger operator of the form $H_t := -\partial_{xx}^2 + V_t(x)$ with the dislocated potential

$$V_t(x) = V(x)\mathbf{1}(x < 0) + V(x-t)\mathbf{1}(x \geq 0),$$

where V is 1-periodic. The map $t \mapsto H_t$ is norm-resolvent continuous and 1-periodic, and we recover periodic models at the endpoints. As mentioned in the introduction, a difficulty with the discrete model is that it is not possible to create such a continuous shift. Our workaround is to introduce a quasi-periodic dislocated model $\tilde{H}^\Sigma(t)$.

The operator $\tilde{H}^\Sigma(t)$ acts on the full space $\ell^2(\mathbb{Z}, \mathbb{C}^N)$ and is defined for $t \in [0, 1]$, by

$$\tilde{H}^\Sigma(t) := \left(\begin{array}{ccc|ccc} \ddots & \ddots & & & & \\ & \ddots & b & a & & \\ & & a^* & b & & \\ \hline & & (1-t)a^* & (1-t)b + t\Sigma & (1-t)a & \\ & & ta^* & (1-t)a^* & b & a \\ & & & & a^* & b & \ddots \\ & & & & & \ddots & \ddots \end{array} \right).$$

This operator is constructed to interpolate linearly between $\tilde{H}^\Sigma(t=0)$ and $\tilde{H}^\Sigma(t=1)$, with

$$\tilde{H}^\Sigma(0) := \left(\begin{array}{ccc|ccc} \ddots & \ddots & & & & \\ & \ddots & b & a & & \\ & & a^* & b & & \\ \hline & & a^* & b & a & \\ & & & a^* & b & \ddots \\ & & & & \ddots & \ddots \end{array} \right), \quad \tilde{H}^\Sigma(1) := \left(\begin{array}{ccc|ccc} \ddots & \ddots & & & & \\ & \ddots & b & a & & \\ & & a^* & b & 0 & a \\ \hline & & & 0 & \Sigma & 0 \\ & & & a^* & 0 & b & a \\ & & & & & a^* & b & \ddots \\ & & & & & & \ddots & \ddots \end{array} \right).$$

The operator $\tilde{H}^\Sigma(0)$ is exactly the periodic Jacobi operator H , and its spectrum is σ_{bulk} . For the operator $\tilde{H}^\Sigma(1)$, we note the following. Let us write $\mathbb{Z} = \{0\} \cup (\mathbb{Z} \setminus \{0\})$, and $\ell^2(\mathbb{Z}, \mathbb{C}^N) = \mathbb{C}^N \oplus \ell^2(\mathbb{Z} \setminus \{0\}, \mathbb{C}^N)$. With respect to this decomposition, we write

$$\forall \Psi \in \ell^2(\mathbb{Z}, \mathbb{C}^N), \quad \Psi = \{\Psi_0\} \oplus \Phi, \quad \text{with} \quad \Phi = (\cdots, \Psi_{-2}, \Psi_{-1}, \Psi_1, \Psi_2, \cdots).$$

Then the operator $\tilde{H}^\Sigma(1)$ acts as

$$\forall \Psi = \{\Psi_0\} \oplus \Phi \in \ell^2(\mathbb{Z}, \mathbb{C}^N), \quad \tilde{H}^\Sigma(1) [\{\Psi_0\} \oplus \Phi] = \{\Sigma \Psi_0\} \oplus H \Phi.$$

In what follows, we will write

$$\tilde{H}^\Sigma(1) = \Sigma \tilde{\oplus} \tilde{H}^\Sigma(0) \tag{13}$$

for such a decomposition. In particular, we have

$$\sigma(\tilde{H}^\Sigma(1)) = \sigma(H) \bigcup \{\Sigma\} = \sigma_{\text{bulk}} \bigcup \{\Sigma\}.$$

In addition, the extra eigenvalue Σ is of multiplicity N . Since the energy E is not in the spectrum of H , and since $\Sigma > E$, it is not in the spectrum of $\tilde{H}^\Sigma(0)$ nor $\tilde{H}^\Sigma(1)$.

Finally, since $\tilde{H}^\Sigma(t)$ is a compact perturbation of H (only a finite number of matrix elements are modified), we have

$$\sigma_{\text{ess}}(\tilde{H}^\Sigma(t)) = \sigma_{\text{ess}}(H) = \sigma_{\text{bulk}},$$

so the essential spectrum is independent of $t \in [0, 1]$. Again, some eigenvalues may appear in these essential gaps. Since E is in such an essential gap, the spectral flow $\text{Sf}(\tilde{H}^\Sigma(t), E, [0, 1])$ is well-defined. Actually, we prove that it equals the one of the right-cut model introduced in the previous section.

Lemma 3.3. *We have*

$$\text{Sf}(H_R^\Sigma(t), E, [0, 1]) = \text{Sf}(\tilde{H}^\Sigma(t), E, [0, 1]).$$

Proof. We consider yet another cut operator $\tilde{K}(t)$, defined by $\tilde{K}(t) = (1-t)\tilde{K}(0) + t\tilde{K}(1)$, with

$$\tilde{K}(0) := \left(\begin{array}{ccc|cc} \ddots & & \ddots & & \\ & \ddots & & 0 & \\ & & 0 & a & 0 \\ \hline & & a^* & 0 & \ddots \\ & & 0 & \ddots & \ddots \end{array} \right), \quad \tilde{K}(1) := \left(\begin{array}{ccc|cc} \ddots & & \ddots & & \\ & \ddots & & 0 & a \\ & & 0 & 0 & \ddots \\ \hline & & 0 & 0 & \ddots \\ & & a^* & \ddots & \ddots \end{array} \right),$$

where all undisplayed elements are null. Note that $\tilde{K}(1) = 0 \oplus \tilde{K}(0)$, hence that $(\tilde{H}^\Sigma - s\tilde{K})(1) = \Sigma \oplus (\tilde{H}^\Sigma - s\tilde{K})(0)$ for all $s \in [0, 1]$. Therefore, by robustness of the spectral flow under compact perturbations, we find that (see Lemma A.11 below)

$$\text{Sf}(\tilde{H}^\Sigma(t), E, [0, 1]) = \text{Sf}(\tilde{H}^\Sigma(t) - \tilde{K}(t), E, [0, 1]).$$

The operator $\tilde{H}(t) - \tilde{K}(t)$ is block diagonal, of the form $\tilde{H}_L^\Sigma(t) \oplus \tilde{H}_R^\Sigma(t)$. This time, the left part is constant, independent of t , hence has a null spectral flow. For the right part, we recover the half Jacobi matrix $H_R^\Sigma(t)$. \square

3.3. Computation of the spectral flow for the dislocated model. The main result of this section is an exact computation of the spectral flow in the dislocated case.

Lemma 3.4. *We have*

$$\text{Sf}(\tilde{H}^\Sigma(t), E, [0, 1]) = -\mathcal{N}(E).$$

This result was first proved in [21, 22] in the case of continuous Schrödinger operators. The proof presented here is similar, but more complete, and uses solely tools from spectral theory.

3.3.1. The finite periodic dislocated model. First, we introduce a finite dimensional version of our dislocated operator. This is the point in the proof where working with periodic Jacobi operators instead of general periodic Hamiltonians becomes easier to write and study. For $\ell \in \mathbb{N}$, we denote by Ω_ℓ the set of ℓ integers centered around 0. Explicitly,

$$\Omega_\ell := \left\{ -\left\lfloor \frac{\ell-1}{2} \right\rfloor, -\left\lfloor \frac{\ell-1}{2} \right\rfloor + 1, \dots, -1, 0, 1, \dots, \left\lfloor \frac{\ell}{2} \right\rfloor - 1, \left\lfloor \frac{\ell}{2} \right\rfloor \right\},$$

so $\Omega_1 = \{0\}$, $\Omega_2 = \{0, 1\}$, $\Omega_3 = \{-1, 0, 1\}$, and so on. In what follows, we identify Ω_ℓ with the torus $\mathbb{Z}/\ell\mathbb{Z}$, but we chose the labelling of Ω_ℓ to display our matrices. For such ℓ with $\ell \geq 5$, we denote by $\tilde{H}_\ell^\Sigma(t)$ a periodic version of the dislocated Hamiltonian $\tilde{H}^\Sigma(t)$. This operator acts on $\ell^2(\Omega_\ell, \mathbb{C}^N)$. In the canonical basis, this is the operator (the bars in the matrix still denote the separation between strictly negative and positive indices)

$$\tilde{H}_\ell^\Sigma(t) := \left(\begin{array}{ccc|cccc} \ddots & & \ddots & & & & \\ & \ddots & & & & & \\ & & b & a & & & \\ & & a^* & b & & & \\ \hline & & (1-t)a^* & (1-t)b+t\Sigma & (1-t)a & & \\ & & ta^* & (1-t)a^* & b & a & \\ & & & & a^* & b & \ddots \\ & & & & & & \ddots & \ddots \\ a & & & & & & & \ddots & \ddots \end{array} \right).$$

Note the presence of a^* (resp. a) in the upper-right (resp. lower-left) corner. Again, this family of matrices is linear in t , and interpolates between $\tilde{H}_\ell^\Sigma(t=0)$ and $\tilde{H}_\ell^\Sigma(t=1)$, with

$$\tilde{H}_\ell^\Sigma(0) := \left(\begin{array}{ccc|ccc} \ddots & & \ddots & & & \\ & \ddots & & & & \\ & & b & a & & \\ & & a^* & b & & \\ \hline & & & a^* & a & \\ & & & b & a & \\ & & & a^* & b & \ddots \\ & a & & & \ddots & \ddots \end{array} \right), \quad \tilde{H}_\ell^\Sigma(1) := \left(\begin{array}{ccc|ccc} \ddots & & \ddots & & & \\ & \ddots & & b & a & \\ & & a^* & b & & \\ \hline & & & 0 & a & \\ & & & 0 & \Sigma & 0 \\ & & & 0 & b & a \\ & & & a^* & 0 & \\ & & & & a^* & b & \ddots \\ & a & & & \ddots & \ddots \end{array} \right).$$

At $t = 0$, the matrix $\tilde{H}_\ell^\Sigma(0)$ is a finite version of the periodic Jacobi matrix H . We will write $H_\ell^\Sigma(0) =: H_\ell$ below to emphasize this point. Its spectrum can be directly computed using Fourier series. Using plane waves with periodicity ℓ , we find (compare with (9))

$$\sigma(H_\ell) = \bigcup_{k \in \Omega_\ell^*} \sigma(a^* e^{-ik} + b + a e^{ik}),$$

with $\Omega_\ell^* := \frac{2\pi}{\ell} \mathbb{Z} \cap \Omega^*$ where we recall that $\Omega^* = (-\pi, \pi]$. In particular, we have $\sigma(H_\ell) \subset \sigma(H)$, and the energy E is not in the spectrum of H_ℓ . Actually, for each of the N Bloch bands $\{\lambda_{j,k}\}_{k \in \Omega^*}$ of H , we can associate the ℓ eigenvalues $\{\lambda_{j,k}\}_{k \in \Omega_\ell^*}$ of H_ℓ .

At $t = 1$, apart from the presence of matrix Σ in the middle, we also recognize a periodic model, and we have a relation of the form (compare with (13))

$$\tilde{H}_\ell^\Sigma(1) = \Sigma \oplus H_{\ell-1}, \quad \text{hence} \quad \sigma(\tilde{H}_\ell^\Sigma(1)) = \sigma(H_{\ell-1}) \cup \{\Sigma\},$$

where Σ is an eigenvalue of multiplicity N .

Lemma 3.5. *For all $\ell \geq 5$, we have $\text{Sf}(\tilde{H}_\ell^\Sigma(t), E, [0, 1]) = -\mathcal{N}(E)$.*

Proof. The map $t \mapsto \tilde{H}_\ell^\Sigma(t)$ is continuous (even linear) in t . So the branches of eigenvalues of these matrices are also continuous in t . At $t = 0$, there are $\ell \mathcal{N}(E)$ eigenvalues of $\tilde{H}_\ell^\Sigma(0)$ below the energy E , and at $t = 1$, there are $(\ell - 1) \mathcal{N}(E)$ eigenvalues of $\tilde{H}_\ell^\Sigma(1)$ below E . This difference implies that the net number of eigenvalues crossing E when t increases to 1 equals $-\mathcal{N}(E)$ \square

Let us recall our analogy of the Grand Hilbert Hotel given in Remark 1.2. In this finite periodic case, there are only a finite number of rooms per floor. The difference between the initial and final number of rooms counts, without ambiguity, the number of eigenvalues that cross from one band to the next.

3.3.2. From the finite dislocated model to the infinite dislocated model. In the previous section, we proved that the spectral flow of the supercell dislocated model \tilde{H}_ℓ^Σ is $-\mathcal{N}(E)$ for all $\ell \geq 5$. In this section, we justify that one may take the limit $\ell \rightarrow \infty$ and deduce that spectral flow of is also $-\mathcal{N}(E)$ for the full dislocated model \tilde{H}^Σ . Throughout this subsection, we drop the superscript Σ , and the *tilde* notation for clarity: we will simply write $H(t)$ and $H_\ell(t)$ for the dislocated models acting on $\ell^2(\mathbb{Z}, \mathbb{C}^N)$ and $\ell^2(\mathbb{Z}, \Omega_\ell)$ respectively. Recall that at $t = 0$, the operators $H(0)$ and $H_\ell(0)$ are periodic, and that

$$\sigma(H_\ell(0)) \subset \sigma_{\text{bulk}}, \quad \sigma(H(0)) = \sigma_{\text{bulk}}.$$

In order to relate the operators H_ℓ and H that act on different Hilbert spaces, we introduce $i_\ell : \mathcal{H}_\ell \rightarrow \mathcal{H}$ for the extension by zero. Explicitly,

$$\forall \Psi \in \mathcal{H}_\ell, \quad \forall n \in \mathbb{Z}, \quad (i_\ell \Psi)_n = \begin{cases} \Psi_n & \text{if } n \in \Omega_\ell, \\ 0 & \text{else} \end{cases},$$

whose adjoint is the restriction operator $i_\ell^* : \mathcal{H} \rightarrow \mathcal{H}_\ell$ given by

$$\forall \Psi \in \mathcal{H}, \forall n \in \Omega_\ell, \quad (i_\ell^* \Psi)_n = \Psi_n.$$

We also introduce a smooth cutoff function $\chi : \mathbb{R} \mapsto [0, 1]$ such that

$$\chi(x) = 1 \quad \forall x \in [-1/4, 1/4], \quad \chi(x) = 0 \quad \forall x \in \mathbb{R} \setminus (-1/3, 1/3)$$

and define χ_ℓ as the multiplication operator by $\chi(\cdot/\ell)$. Note that this function is supported in $[-\ell/3, \ell/3] \subset \Omega_\ell$. For this reason, we abuse notation and use χ_ℓ for multiplication by χ_ℓ from and to \mathcal{H}_ℓ and \mathcal{H} interchangeably. In other words, we identify the operator χ_ℓ in \mathcal{H} with $i_\ell^* \chi_\ell i_\ell$ in \mathcal{H}_ℓ , and $i_\ell^* \chi_\ell$, $\chi_\ell i_\ell$ between \mathcal{H} and \mathcal{H}_ℓ . We will use the following identities throughout this section.

Lemma 3.6. *For all $\ell \geq 12$ and $t \in [0, 1]$ we have,*

- (1) $H(t)\chi_\ell = i_\ell H_\ell(t)\chi_\ell$ and $\chi_\ell H(t) = \chi_\ell H_\ell(t)i_\ell^*$,
- (2) $H(t)(1 - \chi_\ell) = H(0)(1 - \chi_\ell)$ and $H_\ell(t)(1 - \chi_\ell) = H_\ell(0)(1 - \chi_\ell)$,
- (3) *as operators from \mathcal{H} to \mathcal{H}_ℓ , we have*

$$H_\ell(t)\chi_\ell = \chi_\ell H(t) + R_\ell, \quad \text{with } R_\ell \text{ independent of } t \text{ satisfying } \|R_\ell\|_{\text{op}} \leq \frac{C}{\ell}. \quad (14)$$

The first point states that we can replace $H(t)$ with $H_\ell(t)$ in the support of χ_ℓ (the cut-off function erases the boundary conditions). The second point states that outside the support of the cut-off function, the operators are independent of $t \in [0, 1]$. The last point says that one can commute the Hamiltonians with the cut-off operator, up to an error of order $O(\ell^{-1})$.

Proof. For the first point, we note that for all $\Psi \in \mathcal{H}$, the function $\chi_\ell \Psi$ has support in $[-\ell/3, \ell/3]$. Since $H(t)$ is a Jacobi operator, the function $H(t)\chi_\ell \Psi$ has support in $[-\ell/3 - 1, \ell/3 + 1]$, and can be identified with a function in \mathcal{H}_ℓ by applying i_ℓ^* , whenever $\ell \geq 12$. The second relation is the adjoint of the first.

For the second point, we note that $H(t) = H(0) + M(t)$, where $M(t)$ is a finite rank operator with nonzero matrix elements only in the entries $\{-1, 0, 1\}$. So $M(t)(1 - \chi_\ell) = 0$ whenever $\ell \geq 12$, since $\chi_\ell(i) = 1$ for $|i| \leq \ell/4$. The result follows.

For the third point, we first recall that $H(t) = H(0) + M(t)$ and $H_\ell(t) = H_\ell(0) + i_\ell M(t)i_\ell^*$. We already proved that $M_\ell(t)\chi_\ell = \chi_\ell M(t)$ for all $\ell \geq 12$. Next, we find that

$$[H_\ell(0)\chi_\ell - \chi_\ell H(0)]_{ij} = \begin{cases} a(\chi_\ell(n+1) - \chi(n)) & \text{if } (i, j) = (n, n+1) \\ a^*(\chi_\ell(n-1) - \chi(n)) & \text{if } (i, j) = (n, n-1) \\ 0 & \text{else} \end{cases}$$

Note that $|\chi_\ell(n+1) - \chi_\ell(n)| \leq \frac{C}{\ell}$. So

$$R_\ell = H_\ell(t)\chi_\ell - \chi_\ell H(t) = H_\ell(0)\chi_\ell - \chi_\ell H(0) \quad \text{satisfies} \quad \|R_\ell\| \leq 2\|a\|_{\text{op}} \frac{C}{\ell}. \quad \square$$

First, we prove that points in the resolvent set of $H(t)$ are in the resolvent set of $H_\ell(t)$ for sufficiently large values of ℓ .

Lemma 3.7. *There is a constant C , such that, for all $t \in [0, 1]$ and all $\lambda \in \mathbb{C}$ satisfying*

$$\text{dist}(\lambda, \sigma(H(t))) := \varepsilon > 0,$$

we have

$$\text{dist}(\lambda, \sigma(H_\ell(t))) \geq \frac{\varepsilon}{4} \text{ for all } \ell \geq \max(12, C/\varepsilon).$$

Recall that, for a self-adjoint operator A , we have $\text{dist}(\lambda, \sigma(A)) = \|(\lambda - A)^{-1}\|_{\text{op}}^{-1}$.

Proof. Since the essential spectrum of $H(t)$ coincides with σ_{bulk} , we find that $\text{dist}(\lambda, \sigma_{\text{bulk}}) \geq \varepsilon$. Recall that $\sigma(H_\ell(0)) \subset \sigma_{\text{bulk}}$, so in particular $H_\ell(0) - \lambda$ is invertible with $\|(H_\ell(0) - \lambda)^{-1}\|_{\text{op}} \leq \varepsilon^{-1}$.

The same bound holds for $(H(t) - \lambda)^{-1}$. We combine both resolvents to construct an approximate inverse for $H_\ell(t) - \lambda$. Indeed, for any $\ell \geq 12$,

$$\begin{aligned} & (H_\ell(t) - \lambda) \{ \chi_\ell (H(t) - \lambda)^{-1} i_\ell + (1 - \chi_\ell) (H_\ell(0) - \lambda)^{-1} \} \\ &= \chi_\ell i_\ell + R_\ell (H(t) - \lambda)^{-1} i_\ell + (1 - \chi_\ell) - R_\ell (H_\ell(0) - \lambda)^{-1} \\ &= 1 + R_\ell \{ (H(t) - \lambda)^{-1} i_\ell - (H_\ell(0) - \lambda)^{-1} \} := 1 + \mathcal{R}_\ell(t). \end{aligned}$$

We can bound $\mathcal{R}_\ell(t)$ by combining the bounds on the resolvents and on R_ℓ from Lemma 3.6 to obtain

$$\|\mathcal{R}_\ell(t)\|_{\text{op}} \leq \frac{2C}{\varepsilon \ell},$$

Note that the bound is independent of $t \in [0, 1]$. Then, for $\ell \geq C' := \max\{12, \frac{4C}{\varepsilon}\}$, we have $\|\mathcal{R}_\ell(t)\|_{\text{op}} \leq \frac{1}{2}$. We conclude that $H_\ell(t) - \lambda$ is invertible with

$$\begin{aligned} \|(H_\ell(t) - \lambda)^{-1}\|_{\text{op}} &\leq \|\chi_L (H(t) - \lambda)^{-1} i_L + (1 - \chi_L) (H_\ell(0) - \lambda)^{-1}\|_{\text{op}} \|(1 + \mathcal{R}_\ell(t))^{-1}\|_{\text{op}} \\ &\leq \frac{2}{\varepsilon} \frac{1}{1 - \|\mathcal{R}_\ell(t)\|_{\text{op}}} \leq \frac{4}{\varepsilon}. \end{aligned}$$

This is the desired result. \square

To complete the proof, we have to show that the spectral projectors of $H_\ell(t)$ in the gaps of σ_{bulk} converge to spectral projectors of $H(t)$. We record a convenient property of projections.

Lemma 3.8. *Let P be a projector of rank m , and A be a bounded operator such that $\|P - A\|_{\text{op}} < 1$. Then $\text{rank}(A) \geq m$.*

Proof. We have $\|P - PAP\|_{\text{op}} < 1$, so, seen as maps from $E := \text{Ran}(P)$ to itself, we have $\|\mathbb{I}_m - A|_E\| < 1$, which proves that $A|_E$ is full rank on E . So $\text{rank}(A) \geq m$. \square

In what follows, for $\lambda_1 < \lambda_2$, we denote by $P_{(\lambda_1, \lambda_2)}(A)$ the spectral projector of the self-adjoint operator A on the open interval (λ_1, λ_2) . We recall that if λ_1 and λ_2 are not in the spectrum of A , then this spectral projector can be written as the Cauchy contour integral

$$P_{(\lambda_1, \lambda_2)}(A) = \frac{1}{2i\pi} \oint_{\mathcal{C}} \frac{dz}{z - A},$$

where \mathcal{C} is any simple, positively oriented contour in \mathbb{C} enclosing the interval (λ_1, λ_2) and no other portions of the real line. We can take for instance \mathcal{C} the positively oriented circle with center $\frac{1}{2}(\lambda_1 + \lambda_2)$ and radius $\frac{1}{2}(\lambda_2 - \lambda_1)$.

Lemma 3.9. *Fix t and let $\lambda_1 < \lambda_2$ which are not eigenvalues of $H(t)$. Then, for ℓ large enough, we have*

$$\text{rank}(P_{(\lambda_1, \lambda_2)}(H_\ell(t))) = \text{rank}(P_{(\lambda_1, \lambda_2)}(H(t))).$$

Proof. As in the proof of Lemma 3.7, the idea is to localize the resolvent of $H_\ell(t)$ using the cut-off functions χ_ℓ . On the support of χ_ℓ , we compare it with the resolvent of $H(t)$, and outside this support, we compare it with $H_\ell(0)$ (independent of t). Since the interval (λ_1, λ_2) is contained in a gap of σ_{bulk} , the latter part does not contribute to the spectral projection.

To start, let \mathcal{C} be the positively oriented circle as above, which encloses the interval (λ_1, λ_2) . Note that

$$\forall z \in \mathcal{C}, \quad \text{dist}(z, \sigma(H(t))) \geq \max\{\text{dist}(\lambda_1, \sigma(H(t))), \text{dist}(\lambda_2, \sigma(H(t)))\} =: \varepsilon > 0.$$

So, by Lemma 3.7, for $\ell \geq \frac{C}{\varepsilon}$, this contour is also included in the resolvent set of $H_\ell(t)$, and we have the bound

$$\forall z \in \mathcal{C}, \quad \|(z - H_\ell(t))^{-1}\|_{\text{op}} \leq \frac{4}{\varepsilon}, \quad \text{and} \quad \|(z - H_\ell(t))^{-1}\|_{\text{op}} \leq \frac{1}{\varepsilon}.$$

We use the localization function χ_ℓ and $\phi_\ell := \sqrt{1 - \chi_\ell^2}$, such that $\chi_\ell^2 + \phi_\ell^2 = 1$. The support of χ_ℓ is in $[-\ell/3, \ell/3]$, the support of ϕ_ℓ is the complement of $(-\ell/4, \ell/4)$, and there is a constant such that $\|H_\ell(t)\chi_\ell - \chi_\ell H(t)\|_{\text{op}} \leq C/\ell$.

For z on \mathcal{C} , we obtain from Lemma 3.6, (as operators from \mathcal{H} to \mathcal{H}_ℓ)

$$(H_\ell(t) - z)\chi_\ell = \chi_\ell(H(t) - z) + R_\ell.$$

Multiplying this identity by $(H_\ell(t) - z)^{-1}$ on the left and $(H(t) - z)^{-1}$ on the right gives

$$\chi_\ell(H(t) - z)^{-1} = (H_\ell(t) - z)^{-1}\chi_\ell + \mathcal{R}_\ell(z), \quad (15)$$

with $\|\mathcal{R}_\ell(z)\|_{\text{op}} \leq \frac{4}{\varepsilon^2 \ell}$. We also have $(H_\ell(t) - z)^{-1}\phi_\ell^2 = (H_\ell(0) - z)^{-1}\phi_\ell^2$, independent of t . Hence, we obtain

$$\begin{aligned} (H_\ell(t) - z)^{-1} &= (H_\ell(t) - z)^{-1}(\chi_\ell^2 + \phi_\ell^2) \\ &= \chi_\ell(H(t) - z)^{-1}\chi_\ell - \mathcal{R}_\ell(z)\chi_\ell + (H_\ell(0) - z)^{-1}\phi_\ell^2. \end{aligned}$$

Inserting this identity in the Cauchy formula gives

$$P_{(\lambda_1, \lambda_2)}(H_\ell(t)) = \chi_\ell P_{(\lambda_1, \lambda_2)}(H(t))\chi_\ell + P_{(\lambda_1, \lambda_2)}(H_\ell(0))\phi_\ell^2 - \frac{1}{2i\pi} \int_{\mathcal{C}} \mathcal{R}_\ell(z)\chi_\ell dz.$$

Since (λ_1, λ_2) lies in a gap of σ_{bulk} , the second term is actually zero. The last term can be bounded by $2|\mathcal{C}|/(\pi\varepsilon^2\ell)$. Thus, we can find ℓ_0 sufficiently large such that for all $\ell \geq \ell_0$, we have

$$\|P_{(\lambda_1, \lambda_2)}(H_\ell(t)) - \chi_\ell P_{(\lambda_1, \lambda_2)}(H(t))\chi_\ell\|_{\text{op}} < 1.$$

From Lemma 3.9, we conclude that

$$\text{rank}(P_{(\lambda_1, \lambda_2)}(H(t))) \geq \text{rank}(\chi_\ell P_{(\lambda_1, \lambda_2)}(H(t))\chi_\ell) \geq \text{rank}(P_{(\lambda_1, \lambda_2)}(H_\ell(t))).$$

For the opposite inequality, we return to (15) and write this time

$$(H(t) - z)^{-1} = \chi_\ell(H_\ell(t) - z)^{-1}\chi_\ell + \chi_\ell \mathcal{R}_\ell(z) + \phi_\ell^2(H(0) - z)^{-1}.$$

Applying as before the Cauchy formula (the third term vanishes) and Lemma 3.9 gives

$$\text{rank}(P_{(\lambda_1, \lambda_2)}(H_\ell(t))) \geq \text{rank}(\chi_\ell P_{(\lambda_1, \lambda_2)}(H(t))\chi_\ell) \geq \text{rank}(P_{(\lambda_1, \lambda_2)}(H(t)))$$

and completes the proof. \square

We now have all the ingredients to complete the proof of Lemma 3.4 on the spectral flow of $t \mapsto H(t)$.

Proof of Lemma 3.4. Choose a partition $0 = t_0 \leq t_1 \leq \dots \leq t_M = 1$ and positive numbers $(a_i)_{1 \leq i \leq M}$ so that, for all $1 \leq i \leq M$, the projection $P_{(E-a_i, E+a_i)}(H(t))$ is finite rank and $E \pm a_i$ belong to the resolvent set of $H(t)$ for all $t \in [t_{i-1}, t_i]$. We recall in Appendix A that the spectral flow of $t \mapsto H(t)$ is given by

$$\text{Sf}(H(t), E, [0, 1]) = \sum_{i=1}^{M-1} \text{rank } P_{(E+a_i, E+a_{i+1})}(H(t_i)),$$

with the convention that $\text{rank } P_{(\lambda_1, \lambda_2)}(A) = -\text{rank } P_{(\lambda_2, \lambda_1)}(A)$ if $\lambda_2 < \lambda_1$. To use this formula of the spectral flow, we used here that

$$\dim \text{Ker}(H(1) - E) = \dim \text{Ker}(H(0) - E),$$

which comes from the fact that $H(1) = \Sigma \tilde{\oplus} H(0)$.

The hypothesis on $E \pm a_i$ and the continuity of the eigenvalues as a function of t , shows that there is $\varepsilon_i > 0$ such that

$$\forall t \in [t_i, t_{i+1}], \quad \text{dist}(E \pm a_i, \sigma(H(t))) \geq \varepsilon_i.$$

By Lemma 3.7, with $\varepsilon = \min_i \varepsilon_i$ there is ℓ_0 such that, for all $\ell \geq \ell_0$, we have

$$\forall t \in [t_i, t_{i+1}], \quad \text{dist}(E \pm a_i, \sigma(H_\ell(t))) \geq \frac{\varepsilon}{4}.$$

Thus, the partition given by $\{t_i\}_{i=0, \dots, M}$ and the corresponding values a_i are suitable to compute the spectral flow of H_ℓ for all $\ell > \ell_0$. By applying Lemma 3.9, we find a sufficiently large ℓ , such that

$$\text{Ran}(P_{(E+a_i, E+a_{i+1})}(H(t_i))) = \text{Ran}(P_{(E+a_i, E+a_{i+1})}(H_\ell(t_i))) \text{ for } i = 1, \dots, M-1$$

and thus, by using Lemma 3.5,

$$\text{Sf}(H(t), E, [0, 1]) = \text{Sf}(H_\ell(t), E, [0, 1]) = -\mathcal{N}(E). \quad \square$$

4. APPLICATION FOR TWO-DIMENSIONAL MATERIALS

In this section, we apply the previous theory to the case of two-dimensional materials in the tight-binding approximation. Our goal is to describe the spectrum of such materials in the presence of a soft-wall. In the one-dimensional case, we could without loss of generality fix the unit cell to be $[0, 1]$ and the corresponding Fourier variable belongs to $[-\pi, \pi]$. To describe general two-dimensional models, we need the full terminology of solid state physics.

4.1. Reduction to the one-dimensional case.

4.1.1. *Bravais lattices and bulk operators in tight-binding models.* Let us first fix some notation. We consider a \mathbb{L} -periodic crystal, where \mathbb{L} is a Bravais lattice in \mathbb{R}^2 , of the form

$$\mathbb{L} = \mathbf{a}_1\mathbb{Z} \oplus \mathbf{a}_2\mathbb{Z}, \quad \mathbf{a}_1, \mathbf{a}_2 \in \mathbb{R}^2, \quad \det(\mathbf{a}_1, \mathbf{a}_2) \neq 0.$$

We denote by Γ a fundamental cell of the lattice, *i.e.* a subset of \mathbb{R}^2 such that the disjoint union of its \mathbb{L} -translations cover \mathbb{R}^2 : $\bigsqcup_{\mathbf{R} \in \mathbb{L}} \Gamma + \mathbf{R} = \mathbb{R}^2$. A typical choice is $\Gamma = \mathbf{a}_1[0, 1) \oplus \mathbf{a}_2[0, 1)$, but any choice works. We denote by $M \in \mathbb{N}$ the number of atoms in each unit cell Γ . The location of these atoms are $(\mathbf{x}_1, \dots, \mathbf{x}_M)$ with $\mathbf{x}_j \in \Gamma$.

The wave-function is an element $\Psi \in \ell^2(\mathbb{L}, \mathbb{C}^M)$ parametrized as

$$\Psi = (\psi_{\mathbf{R}})_{\mathbf{R} \in \mathbb{L}}, \quad \text{where } \forall \mathbf{R} \in \mathbb{L}, \quad \psi_{\mathbf{R}} = \begin{pmatrix} \psi_{\mathbf{R}}^{(1)} & \psi_{\mathbf{R}}^{(2)} & \dots & \psi_{\mathbf{R}}^{(M)} \end{pmatrix}^T \in \mathbb{C}^M.$$

As noted in the Introduction, one interpretation of this notation is that $\psi_{\mathbf{R}}^{(m)} \in \mathbb{C}$ is the amplitude of the electron on the atom located at $\mathbf{R} + \mathbf{x}_m$. The discrete translation invariance of the perfect, infinite crystal translates in the convolution form of the two-dimensional tight-binding Hamiltonian \mathbf{H} (we use straight letters for two-dimensional operators), of the form

$$\forall \Psi \in \ell^2(\mathbb{L}, \mathbb{C}^M), \quad \forall \mathbf{R} \in \mathbb{L}, \quad (\mathbf{H}\Psi)_{\mathbf{R}} = \sum_{\mathbf{R}' \in \mathbb{L}} h(\mathbf{R}') \Psi_{\mathbf{R}-\mathbf{R}'}, \quad (16)$$

where $h : \mathbb{L} \rightarrow \mathcal{M}_M(\mathbb{C})$ is a family of $M \times M$ matrices satisfying $h(-\mathbf{R}) = h(\mathbf{R})^*$. We assume that $h \in \ell^1(\mathbb{L}, \mathbb{C}^{M \times M})$, which implies as before that \mathbf{H} is a bounded operator on $\ell^2(\mathbb{L}, \mathbb{C}^M)$.

Since \mathbf{H} is a convolution operator, it is diagonal in Fourier basis. As usual in solid state physics, we introduce a pair of reciprocal lattice vectors $\mathbf{a}_1^*, \mathbf{a}_2^*$, that are defined by the relations $\langle \mathbf{a}_i^*, \mathbf{a}_j \rangle_{\mathbb{R}^2} = 2\pi\delta_{ij}$. These vectors generate the reciprocal lattice \mathbb{L}^* , and the natural domain for the Fourier variable is the Brillouin zone $\Gamma^* := \mathbb{R}^2/\mathbb{L}^*$ (seen as a torus). Reasoning as in Section 2.1.1, we find that $\mathcal{F}\mathbf{H}\mathcal{F}^* = \int_{\Gamma^*}^{\oplus} \mathbf{H}_{\mathbf{k}} d\mathbf{k}$, where

$$\forall \mathbf{k} \in \mathbb{R}^2, \quad \mathbf{H}_{\mathbf{k}} = \sum_{\mathbf{R} \in \mathbb{L}} h(\mathbf{R}) e^{-i\mathbf{R} \cdot \mathbf{k}} \in \mathcal{S}_M(\mathbb{C}). \quad (17)$$

The map $\mathbf{k} \mapsto \mathbf{H}_{\mathbf{k}}$ is analytic (it is the sum of a uniformly absolutely convergent series of analytic functions) and \mathbb{L}^* -periodic, so it is enough to describe $\mathbf{H}_{\mathbf{k}}$ on the Brillouin zone $\mathbf{k} \in \Gamma^*$. We denote by $\lambda_{1,\mathbf{k}} \leq \dots \leq \lambda_{M,\mathbf{k}}$ the eigenvalues of $\mathbf{H}_{\mathbf{k}}$, ranked in increasing order. The j -th (two-dimensional) **Bloch band** is the interval $\bigcup_{\mathbf{k} \in \mathbb{R}^2} \{\lambda_{j,\mathbf{k}}\}$, and the spectrum of \mathbf{H} is the union of these M Bloch bands:

$$\sigma_{\text{bulk}} = \sigma(\mathbf{H}) = \bigcup_{\mathbf{k} \in \mathbb{R}^2} \sigma(\mathbf{H}_{\mathbf{k}}) = \bigcup_{j=1}^M \bigcup_{\mathbf{k} \in \Gamma^*} \{\lambda_{j,\mathbf{k}}\}.$$

In the next section, we will add a wall which is constant along the \mathbf{a}_2 -direction (see Section 4.2 below for the case of general angles). This implies that the model with the wall is still periodic in

the \mathbf{a}_2 -direction. In particular, we may perform a partial Fourier transform in this direction. It is useful at this point to introduce the one-dimensional lattices

$$\begin{aligned} \mathbb{L}_1 &:= \mathbf{a}_1 \mathbb{Z}, & \mathbb{L}_2 &:= \mathbf{a}_2 \mathbb{Z}, & \text{so that} & & \mathbb{L} &= \mathbb{L}_1 \oplus \mathbb{L}_2, \\ \mathbb{L}_1^* &:= \mathbf{a}_1^* \mathbb{Z}, & \mathbb{L}_2^* &:= \mathbf{a}_2^* \mathbb{Z}, & \text{so that} & & \mathbb{L}^* &= \mathbb{L}_1^* \oplus \mathbb{L}_2^*. \end{aligned}$$

We also denote by $\Gamma_2^* := (\mathbf{a}_2^* \mathbb{R}) / \mathbb{L}_2^*$ the Brillouin zone of the \mathbb{L}_2 lattice, seen as a torus/line in the two-dimensional space \mathbb{R}^2 , in the sense that we keep the orientation of this line along the \mathbf{a}_2 -direction. We write $\mathbf{k}_2 \in \Gamma_2^*$ for the Fourier variable in this direction. In the literature, it is often identified with the one-dimensional real torus/line, with the identification $\mathbf{k}_2 = k_2 \frac{\mathbf{a}_2^*}{|\mathbf{a}_2^*|}$ where $k_2 = |\mathbf{k}_2| \in \mathbb{R} / |\mathbf{a}_2^*| \mathbb{Z}$.

With these conventions, the partial Fourier transform is $\mathcal{F}_2 : \ell^2(\mathbb{L}, \mathbb{C}^M) \rightarrow L^2(\mathbb{L}_1 \times \Gamma_2^*, \mathbb{C}^M)$ defined by

$$\forall (\mathbf{R}_1, \mathbf{k}_2) \in \mathbb{L}_1 \times \Gamma_2^*, \quad (\mathcal{F}_2[\Psi])(\mathbf{R}_1, \mathbf{k}_2) := \frac{1}{\sqrt{|\Gamma_2^*|}} \sum_{\mathbf{R}_2 \in \mathbb{L}_2} \Psi_{\mathbf{R}_1 + \mathbf{R}_2} e^{-i\mathbf{k}_2 \cdot \mathbf{R}_2}. \quad (18)$$

We obtain that $\mathcal{F}_2 H \mathcal{F}_2^* = \int_{\Gamma_2^*}^{\oplus} H_{\mathbf{k}_2} d\mathbf{k}_2$, where, for all $\mathbf{k}_2 \in \Gamma_2^*$, $H_{\mathbf{k}_2}$ is an operator acting on the one-dimensional lattice $\ell^2(\mathbb{L}_1, \mathbb{C}^M)$, of the form

$$\forall \Psi \in \ell^2(\mathbb{L}_1, \mathbb{C}^M), \quad \forall \mathbf{R}_1 \in \mathbb{L}_1 \quad (H_{\mathbf{k}_2} \Psi)_{\mathbf{R}_1} = \sum_{\mathbf{R}'_1 \in \mathbb{L}_1} h_{\mathbf{k}_2}(\mathbf{R}'_1) \Psi_{\mathbf{R}_1 - \mathbf{R}'_1},$$

where the kernel $h_{\mathbf{k}_2}$ is

$$\forall \mathbf{R}_1 \in \mathbb{L}_1, \quad h_{\mathbf{k}_2}(\mathbf{R}_1) := \sum_{\mathbf{R}_2 \in \mathbb{L}_2} h(\mathbf{R}_1 + \mathbf{R}_2) e^{-i\mathbf{k}_2 \cdot \mathbf{R}_2}. \quad (19)$$

Note that the series is convergent and the resulting one-dimensional kernel satisfies the hypothesis of the previous section, since $h \in \ell^1(\mathbb{L})$ implies $h_{\mathbf{k}_2} \in \ell^1(\mathbb{L}_1)$ by Fubini's Theorem.

In what follows, we fix $\mathbf{k}_2 \in \Gamma_2^*$, and study the one-dimensional periodic operator $H_{\mathbf{k}_2}$, and its soft-wall counterpart $H_{\mathbf{k}_2}^\sharp(t)$. The spectrum of $H_{\mathbf{k}_2}$ is purely essential, composed of M (one-dimensional) Bloch bands. It is the union of the spectra of $(H_{\mathbf{k}_2})_{\mathbf{k}_1}$, defined as (compare with (4))

$$\forall \mathbf{k}_1 \in \Gamma_1^*, \quad (H_{\mathbf{k}_2})_{\mathbf{k}_1} := \sum_{\mathbf{R}_1 \in \mathbb{L}_1} h_{\mathbf{k}_2}(\mathbf{R}_1) e^{-i\mathbf{k}_1 \cdot \mathbf{R}_1}.$$

Together with (19), we get that

$$(H_{\mathbf{k}_2})_{\mathbf{k}_1} = \sum_{\mathbf{R}_1 \in \mathbb{L}_1} \sum_{\mathbf{R}_2 \in \mathbb{L}_2} h(\mathbf{R}_1 + \mathbf{R}_2) e^{-i\mathbf{k}_2 \cdot \mathbf{R}_2 - i\mathbf{k}_1 \cdot \mathbf{R}_1} = \sum_{\mathbf{R} \in \mathbb{L}} h(\mathbf{R}) e^{-i\mathbf{k} \cdot \mathbf{R}} = H_{\mathbf{k}_1 + \mathbf{k}_2}.$$

We deduce that

$$\sigma(H_{\mathbf{k}_2}) = \bigcup_{\mathbf{k}_1 \in \Gamma_1^*} \sigma(h_{\mathbf{k}_2}(\mathbf{k}_1)) = \bigcup_{\mathbf{k}_1 \in \Gamma_1^*} \sigma(H_{\mathbf{k}_1 + \mathbf{k}_2}) = \bigcup_{\mathbf{k}_1 \in \mathbf{a}_1^* \mathbb{R}} \sigma(H_{\mathbf{k}_1 + \mathbf{k}_2}). \quad (20)$$

One should think of this formula as follows: the spectrum of $H_{\mathbf{k}_2}$ is the *projection* of the two-dimensional bands (the spectra of $H_{\mathbf{k}}$) on the $\Gamma_2^* \approx \mathbf{a}_2^* \mathbb{R}$ line, where the projection is along the \mathbf{a}_1^* -direction. Note that \mathbf{a}_1^* is the direction orthogonal to the \mathbf{a}_2 vector (which will be the direction of the wall). We extend this formula to the case of general angles below.

4.1.2. Soft walls parallel to a lattice vector. We now add a soft wall potential. We will choose our wall aligned with the \mathbf{a}_2 vector (see Section 4.2 below for other *commensurate* directions). To do so, we introduce the normalized vector $\mathbf{a}_2^\perp := \frac{\mathbf{a}_1^*}{|\mathbf{a}_1^*|}$. This vector satisfies $\mathbf{a}_2^\perp \cdot \mathbf{a}_2 = 0$ and $\mathbf{a}_2^\perp \cdot \mathbf{a}_1 = \frac{2\pi}{|\mathbf{a}_1^*|}$. We consider a two-dimensional soft wall potential $w : \mathbb{R}^2 \rightarrow \mathcal{S}_M(\mathbb{C})$ of the form

$$\forall \mathbf{x} \in \mathbb{R}^2, \quad w(\mathbf{x}) = w_*(\mathbf{a}_2^\perp \cdot \mathbf{x}),$$

where $w_* : \mathbb{R} \mapsto \mathcal{S}_M(\mathbb{C})$ is a one-dimensional Lipschitz soft wall potential as in Section 2.1.2. Note that $w(\mathbf{x} + \lambda \mathbf{a}_2) = w(\mathbf{x})$, so this wall is constant along the \mathbf{a}_2 direction. In addition, since \mathbf{a}_2^\perp

is normalized, this potential has the same Lipschitz constant as w_1 . To introduce a dislocation parameter $t \in \mathbb{R}$, we set

$$w_t(\mathbf{x}) := w(\mathbf{x} - t\mathbf{a}_1) = w_* (\mathbf{a}_2^\perp \cdot (\mathbf{x} - t\mathbf{a}_1)) = w_* \left(\mathbf{a}_2^\perp \cdot \mathbf{x} - t \frac{2\pi}{\|\mathbf{a}_1^*\|} \right). \quad (21)$$

The corresponding operator $W(t)$ acting on $\ell^2(\mathbb{L}, \mathbb{C}^M)$ is the block-diagonal operator

$$\forall \Psi \in \ell^2(\mathbb{L}, \mathbb{C}^M), \quad \forall \mathbf{R} \in \mathbb{L}, \quad (W(t)\Psi)_{\mathbf{R}} = w_t(\mathbf{R})\Psi_{\mathbf{R}}.$$

For a physical crystal subject to a scalar potential v_* which is constant in the \mathbf{a}_2 -direction, one would consider a diagonal potential of the form

$$w_t(\mathbf{R}) = \text{diag} (v_*(\mathbf{a}_2^\perp \cdot (\mathbf{R} - t\mathbf{a}_1 + \mathbf{x}_1)), \dots, v_*(\mathbf{a}_2^\perp \cdot (\mathbf{R} - t\mathbf{a}_1 + \mathbf{x}_M))), \quad (22)$$

where we recall that $\mathbf{x}_1, \dots, \mathbf{x}_M$ are the positions of the atoms with respect to the center of the unit cell. Note that if $\mathbf{R} = n\mathbf{a}_1 + m\mathbf{a}_2$, then $\mathbf{a}_2^\perp \cdot \mathbf{R} = n\mathbf{a}_2^\perp \cdot \mathbf{a}_1$.

Finally, the soft-wall model is the operator

$$H^\sharp(t) = H + W(t), \quad \text{with domain } \mathcal{D}(W) \subset \ell^2(\mathbb{Z}^2, \mathbb{C}^M).$$

This operator is periodic in the \mathbf{a}_2 -direction. After the partial Fourier transform in this direction, we obtain that $\mathcal{F}_2 H_t^\sharp \mathcal{F}_2 = \int_{\Gamma_2^*}^\oplus H_{\mathbf{k}_2}^\sharp(t) d\mathbf{k}_2$ where $H_{\mathbf{k}_2}^\sharp(t)$ acts on $\ell^2(\mathbb{Z}, \mathbb{C}^M)$ with

$$H_{\mathbf{k}_2}^\sharp(t) = H_{\mathbf{k}_2} + W(t).$$

We recover the soft-wall described in Section 2.1.2: the normalization for t in (21) has been chosen so that when t moves from 0 to 1, the wall shifts by the vector \mathbf{a}_1 . We can now apply the previous results to this case.

4.1.3. Edge spectrum in the two-dimensional setting. For an energy $E \in \mathbb{R} \setminus \sigma_{\text{bulk}} := \sigma(H)$, we denote by $\mathcal{N}(E)$ the number of (two-dimensional) Bloch bands of the two-dimensional bulk operator H below E . It is the only integer for which

$$\forall \mathbf{k} \in \mathbb{R}^2, \quad \lambda_{\mathcal{N}(E), \mathbf{k}} < E < \lambda_{\mathcal{N}(E)+1, \mathbf{k}},$$

where we recall that $\lambda_{1, \mathbf{k}} \leq \dots \leq \lambda_{M, \mathbf{k}}$ are the eigenvalues of the $M \times M$ matrix $H(\mathbf{k})$ defined in (17). Similarly, for $\mathbf{k}_2 \in \Gamma_2^*$, and for an energy $E \in \mathbb{R} \setminus \sigma(H_{\mathbf{k}_2})$, we denote by $\mathcal{N}_{\mathbf{k}_2}(E)$ the number of (one-dimensional) Bloch bands of $H_{\mathbf{k}_2}$ below E . It is the integer for which

$$\forall \mathbf{k}_1 \in \mathbf{a}_1^* \mathbb{R}, \quad \lambda_{\mathcal{N}(E), \mathbf{k}_1 + \mathbf{k}_2} < E < \lambda_{\mathcal{N}(E)+1, \mathbf{k}_1 + \mathbf{k}_2}.$$

If $E \in \mathbb{R} \setminus \sigma_{\text{bulk}}$ is in the essential gap of the full two-dimensional operator $H_{\mathbf{k}}$, then, we have $\mathcal{N}_{\mathbf{k}_2}(E) = \mathcal{N}(E)$ for all $\mathbf{k}_2 \in \Gamma_2^*$. However, it may happen that an energy E belongs to the essential gap of $H_{\mathbf{k}_2}$ for *some* values of \mathbf{k}_2 , and is not in an essential gap of the full operator H . In this case, $\mathcal{N}_{\mathbf{k}_2}(E)$ may be well-defined, but not $\mathcal{N}(E)$. This happens for instance in the Wallace model for graphene (see Section 4.3 below).

We can now state our result in the two-dimensional case. It is a straightforward application of Proposition 2.4 and Theorem 1.1.

Theorem 4.1. *Assume that $w_1 : \mathbb{R} \mapsto \mathcal{S}_M$ is a Lipschitz soft-wall. Then, with the previous notation,*

- (1) *For all $\mathbf{k}_2 \in \Gamma_2^*$, and all $t \in \mathbb{R}$, the operator $H_{\mathbf{k}_2}^\sharp(t)$ is a well-defined self-adjoint operator whose domain is independent of \mathbf{k}_2 and t and given by*

$$\mathcal{D} := \{ \Psi \in \ell^2(\mathbb{L}_1, \mathbb{C}^M), \quad W_{t=0} \Psi \in \ell^2(\mathbb{L}_1, \mathbb{C}^M) \}.$$

- (2) *The map $\Gamma_2^* \times \mathbb{R} \ni (\mathbf{k}_2, t) \mapsto H_{\mathbf{k}_2}^\sharp(t)$ is norm-resolvent continuous and 1-quasi-periodic in t .*
- (3) *For all fixed $\mathbf{k}_2 \in \Gamma_2^*$, the spectrum $t \mapsto \sigma(H_{\mathbf{k}_2}^\sharp(t))$ is 1-periodic in t . The essential spectrum $\sigma_{\text{ess}}(H_{\mathbf{k}_2}^\sharp(t))$ is independent of t , and equals $\sigma(H_{\mathbf{k}_2})$ described in (20).*

(4) For all fixed $\mathbf{k}_2 \in \Gamma_2^*$, and for all $E \in \mathbb{R} \setminus \sigma(H_{\mathbf{k}_2})$, we have

$$\text{Sf} \left(H_{\mathbf{k}_2}^\sharp(t), E, [0, 1] \right) = -\mathcal{N}_{\mathbf{k}_2}(E).$$

Concerning the spectrum at fixed $t = t_0$, we can apply Theorem 1.3. We first make the observation that if $w(\cdot)$ is ν -Lipschitz, then, for all $\mathbf{x} \in \mathbb{R}^2$, the map $t \mapsto w_t(\mathbf{x})$ is $\nu \frac{|\Gamma|}{\|\mathbf{a}_2\|}$ -Lipschitz. Indeed, we have, using the classical identity $\|\mathbf{a}_1^*\| = 2\pi\|\mathbf{a}_2\||\Gamma|^{-1}$, that

$$|\tilde{w}_t(\mathbf{x}) - \tilde{w}_{t'}(\mathbf{x})| = \left| w \left(\mathbf{a}_2^\perp \cdot \mathbf{x} - t \frac{2\pi}{\|\mathbf{a}_1^*\|} \right) - w \left(\mathbf{a}_2^\perp \cdot \mathbf{x} - t' \frac{2\pi}{\|\mathbf{a}_1^*\|} \right) \right| \leq \nu \frac{2\pi}{\|\mathbf{a}_1^*\|} |t - t'| = \nu \frac{|\Gamma|}{\|\mathbf{a}_2\|} |t - t'|.$$

In particular, the maps $t \mapsto W_t$ and $t \mapsto H_{\mathbf{k}_2}^\sharp(t)$ are also $\nu \frac{|\Gamma|}{\|\mathbf{a}_2\|}$ -Lipschitz. We obtain the following corollary of Theorem 1.3.

Theorem 4.2. *Let $w : \mathbb{R} \mapsto \mathcal{S}_N$ be a soft-wall which is ν -Lipschitz, for some $\nu > 0$. Then, for all $\mathbf{k}_2 \in \Gamma_2^*$, all energy E belonging to an essential gap of width $g(E) \geq \nu|\Gamma|\|\mathbf{a}_2\|^{-1}$ of $H_{\mathbf{k}_2}$, and all $t_0 \in \mathbb{R}$, the operator $H_{\mathbf{k}_2}^\sharp(t_0)$ has at least $\mathcal{N}(E)$ eigenvalues in each interval of the form $(\lambda, \lambda + \nu|\Gamma|\|\mathbf{a}_2\|^{-1}]$ in this gap.*

In particular, there are at least $\left\lfloor \frac{g(E)\|\mathbf{a}_2\|}{\nu|\Gamma|} \right\rfloor \mathcal{N}_{\mathbf{k}_2}(E)$ eigenvalues in this gap.

We skip its proof, as it is similar to the one of Theorem 1.3. This time, the density of eigenvalues is of order $\frac{\nu|\Gamma|}{\mathcal{N}_{\mathbf{k}_2}(E)\|\mathbf{a}_2\|}$.

4.2. Walls in other directions. we now give one possible way to extend our result to walls which are rotated by any commensurable angle. In the case of incommensurate angles, one can follow [17] to prove that *all essential bulk gaps are filled with edge spectrum*, for all values of t .

We will show that a wall along any commensurable angle can be cast in the previous framework by increasing the size of the unit cell. For two co-prime integers n, m with $n \neq 0$ and $m \neq 0$, we define the new vectors

$$\tilde{\mathbf{a}}_1 := n\mathbf{a}_1, \quad \text{and} \quad \tilde{\mathbf{a}}_2 := n\mathbf{a}_1 + m\mathbf{a}_2. \quad (23)$$

In this section, the wall will be aligned with the vector $\tilde{\mathbf{a}}_2$, and move along the $\tilde{\mathbf{a}}_1$ -direction (which is also the \mathbf{a}_1 -direction). Varying n and m allows to describe all commensurable directions for the wall, except for the \mathbf{a}_1 and \mathbf{a}_2 -directions (which were studied in the previous section).

These two vectors generate a new lattice $\tilde{\mathbb{L}}$, which is a sublattice of the original \mathbb{L} . We denote by $\tilde{\Gamma}$ a corresponding unit cell (supercell). The number of atoms per unit cell is now

$$\tilde{M} = |nm|M.$$

We consider the tight-binding Hamiltonian $\tilde{\mathbf{H}}$ as the representation of the original \mathbf{H} with $\tilde{\Gamma}$ as unit cell. Note that the new kernel $\tilde{\mathbf{h}}$ is now a function from $\tilde{\mathbb{L}}$ to $\mathbb{C}^{\tilde{M} \times \tilde{M}}$.

4.2.1. Bulk spectrum. The spectrum of the bulk Hamiltonian is identical in both frameworks, but written in the Fourier decomposition for the $\tilde{\mathbb{L}}$ lattice, it consists of $|nm|$ -times more bands on a $|nm|$ -times smaller Brillouin zone: a single band for the original Hamiltonian \mathbf{H} corresponds to $|nm|$ bands of the *supercell Hamiltonian* $\tilde{\mathbf{H}}$. To make things concrete, we write $L = |nm|$ and label the L points of $\mathbb{L} \cap \tilde{\Gamma}$ as $\mathbf{y}_1, \dots, \mathbf{y}_L$. We then define $\mathcal{S} : \ell^2(\mathbb{L}, \mathbb{C}^M) \mapsto \ell^2(\tilde{\mathbb{L}}, (\mathbb{C}^M)^L)$ by

$$(\mathcal{S}\Psi)(\mathbf{R}) = (\Psi(\mathbf{R} + \mathbf{y}_1), \dots, \Psi(\mathbf{R} + \mathbf{y}_L))^\top$$

With this transformation, $\tilde{\mathbf{H}} := \mathcal{S}\mathbf{H}\mathcal{S}^*$ acts as

$$(\tilde{\mathbf{H}}\Phi)(\mathbf{R}) = \sum_{\mathbf{R}' \in \tilde{\mathbb{L}}} \tilde{\mathbf{h}}(\mathbf{R}') \Phi_{\mathbf{R}-\mathbf{R}'} \quad \text{where } \tilde{\mathbf{h}}(\mathbf{R}')_{ij} = \mathbf{h}(\mathbf{R}' - \mathbf{y}_i + \mathbf{y}_j).$$

Then, a computation shows that the dual lattice of $\tilde{\mathbb{L}}$ is $\tilde{\mathbb{L}}^* := \tilde{\mathbf{a}}_1^* \mathbb{Z} \oplus \tilde{\mathbf{a}}_2^* \mathbb{Z}$, with

$$\tilde{\mathbf{a}}_1^* = \frac{\mathbf{a}_1^*}{n} - \frac{\mathbf{a}_2^*}{m} \quad \tilde{\mathbf{a}}_2^* = \frac{\mathbf{a}_2^*}{m}. \quad (24)$$

This time, it is the dual lattice \mathbb{L}^* which is a sublattice of $\tilde{\mathbb{L}}^*$. The corresponding Brillouin zone $\tilde{\Gamma}^* := \mathbb{R}^2 / \tilde{\mathbb{L}}^*$ has an area $|\tilde{\Gamma}^*| = \frac{1}{|nm|} |\Gamma^*|$. The operator \tilde{H} is again a convolution, and we denote by $\tilde{H}(\mathbf{k})$ the corresponding Fourier fibers of the operators. The map $\mathbf{k} \mapsto \tilde{H}(\mathbf{k})$ is smooth and $\tilde{\mathbb{L}}^*$ -periodic. We describe this relation more precisely in this short Lemma.

Lemma 4.3. *We have*

$$\sigma(\tilde{H}(\mathbf{k})) = \bigcup_{\tilde{\mathbf{K}} \in \tilde{\mathbb{L}}^* \cap \Gamma^*} \sigma(H(\mathbf{k} + \tilde{\mathbf{K}})) = \bigcup_{\tilde{\mathbf{K}} \in \tilde{\mathbb{L}}^*} \sigma(H(\mathbf{k} + \tilde{\mathbf{K}})).$$

Proof. This result is classical but we provide a simple proof. Recall the definition

$$\tilde{H}_{\mathbf{k}} = \sum_{\mathbf{R} \in \tilde{\mathbb{L}}} \tilde{h}(\mathbf{R}) e^{-i\mathbf{R} \cdot \mathbf{k}} \in \mathcal{S}_{LM}(\mathbb{C}).$$

We fix $\mathbf{k} \in \mathbb{R}^2$ (or in the Brillouin zone $\mathbb{R}^2 / \tilde{\mathbb{L}}^*$) and compute its spectrum. To this end, for some $u \in \mathbb{C}^M$ and $\mathbf{K} \in \tilde{\mathbb{L}}^*$, we define

$$u_{\mathbf{K}} := \left(e^{-iy_1 \cdot (\mathbf{k} + \mathbf{K})} u, \dots, e^{-iy_L \cdot (\mathbf{k} + \mathbf{K})} u \right)^\top$$

and compute, taking advantage of the periodicity of $\tilde{H}_{\mathbf{k}}$,

$$\begin{aligned} (\tilde{H}_{\mathbf{k}} u_{\mathbf{K}})_i &= (\tilde{H}_{\mathbf{k} + \mathbf{K}} u_{\mathbf{K}})_i = \sum_{\mathbf{R} \in \tilde{\mathbb{L}}} e^{-i\mathbf{R} \cdot (\mathbf{k} + \mathbf{K})} (\tilde{h}(\mathbf{R}) u_{\mathbf{K}})_i \\ &= \sum_{\mathbf{R} \in \tilde{\mathbb{L}}} e^{-i\mathbf{R} \cdot (\mathbf{k} + \mathbf{K})} \sum_{j=1}^L h(\mathbf{R} - \mathbf{y}_i + \mathbf{y}_j) e^{-iy_j \cdot (\mathbf{k} + \mathbf{K})} u. \end{aligned}$$

Relabeling $\mathbf{R}' := \mathbf{R} - \mathbf{y}_i + \mathbf{y}_j$, we note that this variable runs over all sites of the original lattice \mathbb{L} , so we obtain finally

$$(\tilde{H}_{\mathbf{k}} u_{\mathbf{K}})_i = e^{-iy_i \cdot (\mathbf{k} + \mathbf{K})} \sum_{\mathbf{R}' \in \mathbb{L}} e^{-i\mathbf{R}' \cdot (\mathbf{k} + \mathbf{K})} h(\mathbf{R}') u = e^{-iy_i \cdot (\mathbf{k} + \mathbf{K})} H_{\mathbf{k} + \mathbf{K}} u.$$

If u is an eigenvector of $H_{\mathbf{k} + \mathbf{K}}$, then $u_{\mathbf{K}}$ is an eigenvector of $\tilde{H}_{\mathbf{k}}$ with the same eigenvalue, for all $\mathbf{K} \in \tilde{\mathbb{L}}^*$. In addition, the eigenvectors $u_{\mathbf{K}}$ are linearly independent for $\mathbf{K} \in \tilde{\mathbb{L}}^* / \mathbb{L}^*$, so we have obtained the LM eigenvalues of the supercell Hamiltonian $\tilde{H}(\mathbf{k})$, and the result follows. \square

When we perform a partial Fourier transform of \tilde{H} in the $\tilde{\mathbf{a}}_2$ -direction, and obtain the new family $\tilde{H}_{\tilde{\mathbf{k}}_2}$ with $\tilde{\mathbf{k}}_2 \in \tilde{\Gamma}_2^*$.

Lemma 4.4. *We have*

$$\sigma(\tilde{H}_{\tilde{\mathbf{k}}_2}) = \bigcup_{\tilde{\mathbf{k}}_1 \in \tilde{\mathbf{a}}_1^* \mathbb{R}} \sigma(\tilde{H}(\tilde{\mathbf{k}}_1 + \tilde{\mathbf{k}}_2)).$$

In other words, the spectrum of $\tilde{H}_{\tilde{\mathbf{k}}_2}$ is again the projection of the spectra of initial operator $H_{\mathbf{k}}$ along the \mathbf{a}_1^* -direction (which is the direction orthogonal to the wall). It is therefore quite easy to compute the (essential) spectrum of the one-dimensional bulk operator $\tilde{H}_{\tilde{\mathbf{k}}_2}$ for any angle: it is a projection of the two-dimensional Bloch bands of the bulk operator $H_{\mathbf{k}}$ (which is independent of the angle) along a particular direction. Figure 5 illustrates this phenomenon for the Wallace model.

Proof. As in (20), we find that

$$\sigma(\tilde{H}_{\tilde{\mathbf{k}}_2}) = \bigcup_{\tilde{\mathbf{k}}_1 \in \tilde{\Gamma}_1^*} \sigma(\tilde{H}(\tilde{\mathbf{k}}_1 + \tilde{\mathbf{k}}_2))$$

Together with Lemma 4.3, we deduce that

$$\sigma(\tilde{H}_{\tilde{\mathbf{k}}_2}) = \bigcup_{\tilde{\mathbf{K}} \in \tilde{\mathbb{L}}^*} \bigcup_{\tilde{\mathbf{k}}_1 \in \tilde{\Gamma}_1^*} \sigma(\tilde{H}(\tilde{\mathbf{k}}_1 + \tilde{\mathbf{k}}_2 + \tilde{\mathbf{K}})) = \bigcup_{\tilde{\mathbf{k}}_1 \in \tilde{\mathbf{a}}_1^* \mathbb{R}} \bigcup_{\tilde{\mathbf{K}}_2 \in \tilde{\mathbf{a}}_2^* \mathbb{Z}} \sigma(\tilde{H}(\tilde{\mathbf{k}}_1 + \tilde{\mathbf{k}}_2 + \tilde{\mathbf{K}}_2^*)).$$

It remains to prove that the union in $\tilde{\mathbf{K}}_2^*$ can be dropped. Recall that we assume that n and m are coprime. Let $p, q \in \mathbb{Z}^2$ so that $pn + qm = 1$. We have, using (24),

$$\mathbf{H}(\mathbf{k} - pn\tilde{\mathbf{a}}_1^*) = \mathbf{H}\left(\mathbf{k} - p\mathbf{a}_1^* + \frac{pn}{m}\mathbf{a}_2^*\right) = \mathbf{H}\left(\mathbf{k} - p\mathbf{a}_1^* - q\mathbf{a}_2^* + \frac{1}{m}\mathbf{a}_2^*\right) = \mathbf{H}(\mathbf{k} + \tilde{\mathbf{a}}_2^*),$$

where we used the \mathbb{L} -periodicity of $\mathbf{k} \mapsto \mathbf{H}(\mathbf{k})$ in the last equality. This proves that any integer shift in the $\tilde{\mathbf{a}}_2^*$ -direction can be implemented as another shift in the $\tilde{\mathbf{a}}_1^*$ -direction. The result follows. \square

4.2.2. Spectral flow for the edge Hamiltonian with general angles. We denote by $\tilde{\mathbf{H}}^\sharp(t)$ the tight-binding model with a soft wall defined as in the previous section, but now with $\tilde{\mathbf{a}}_2$. Applying Theorem 4.2 to this case results in

Theorem 4.5. *Let $w : \mathbb{R} \mapsto \mathcal{S}_N$ be a soft-wall which is ν -Lipschitz, for some $\nu > 0$. If E belongs to an essential gap of width $g(E) \geq \nu$, then for all $t_0 \in \mathbb{R}$ the operator $\tilde{H}^\sharp(t_0)_{\tilde{\mathbf{k}}_2}$ has at least $\mathcal{N}(E)$ eigenvalues in each interval of the form $(\lambda, \lambda + \nu|\Gamma|/\|\tilde{\mathbf{a}}_2\|)$ in this gap.*

Note that the density of edge states is of order $\mathcal{N}(E)\|\tilde{\mathbf{a}}_2\|/(\nu|\Gamma|)$. When the cut becomes close to incommensurate, in the sense that $\|\tilde{\mathbf{a}}_2\|$ becomes large, then there are numerous edge states for each value of $\tilde{\mathbf{k}}_2$.

Proof. According to Theorem 4.1,

$$\text{Sf}\left(\tilde{H}_{\tilde{\mathbf{k}}_2}^\sharp(t), E, [0, 1]\right) = -\mathcal{N}_{\tilde{\mathbf{H}}}(E).$$

Each Bloch band in the supercell framework corresponds to L Bloch bands of the original Hamiltonian, so we have $\mathcal{N}_{\tilde{\mathbf{H}}}(E) = L\mathcal{N}_{\mathbf{H}}(E)$. On the other hand, we claim that the spectrum of $\tilde{H}_{\tilde{\mathbf{k}}_2}^\sharp(t)$ is periodic in t with period $1/L$. This can be seen as follows.

Recall that n, m are coprimes, and let $p, q \in \mathbb{Z}$ be such that $pn + qm = 1$ as before. Then, we have $\frac{1}{nm} = \frac{p}{n} + \frac{q}{m}$. This gives,

$$\tilde{w}_{\frac{1}{nm}}(\mathbf{x}) = w_*\left(\tilde{\mathbf{a}}_2^\perp \cdot \left(\mathbf{x} - \frac{1}{nm}\tilde{\mathbf{a}}_1\right)\right) = \tilde{w}\left(\tilde{\mathbf{a}}_2^\perp \cdot \left(\mathbf{x} - \frac{1}{nm}\tilde{\mathbf{a}}_1 + \frac{1}{m}\tilde{\mathbf{a}}_2\right)\right) = \tilde{w}\left(\tilde{\mathbf{a}}_2^\perp \cdot (\mathbf{x} + \mathbf{a}_2)\right),$$

so $\tilde{w}_{\frac{1}{nm}}(\mathbf{x}) = \tilde{w}_0(\mathbf{x} + \mathbf{a}_2)$. After a shift of the wall by $t = \frac{1}{nm}$, we recover the initial model, translated by $-\mathbf{a}_2$. This proves our claim. We conclude that

$$\text{Sf}\left(\tilde{H}_{\tilde{\mathbf{k}}_2}^\sharp(t), E, \left[0, \frac{1}{L}\right]\right) = \frac{1}{L}\text{Sf}\left(\tilde{H}_{\tilde{\mathbf{k}}_2}^\sharp(t), E, [0, 1]\right) = -\mathcal{N}_{\mathbf{H}}(E).$$

Recalling that the eigenvalue branches for $t \mapsto \tilde{\mathbf{H}}_{\tilde{\mathbf{k}}_2}^\sharp(t)$ are Lipschitz with constant $\nu|\tilde{\Gamma}|/\|\tilde{\mathbf{a}}_2\| = \nu L\Gamma/\|\tilde{\mathbf{a}}_2\|$ and mimicking the proof of Theorem 1.3 gives the result. \square

4.3. Example : the Wallace model for graphene. We now apply the previous results in the case of graphene, within the Wallace approximation. We consider three different angles, and compute the edge spectral flow in these three cases.

4.3.1. The Wallace model. Let us start by describing the bulk spectrum of graphene. Graphene has a honeycomb lattice structure, which is the triangular Bravais lattice, with two atoms per unit cell. As basis vectors, we may chose

$$\mathbb{L} = \mathbf{a}_1\mathbb{Z} \oplus \mathbf{a}_2\mathbb{Z} \quad \text{with} \quad \mathbf{a}_1 = \frac{a_0}{2} \begin{pmatrix} 1 \\ -\sqrt{3} \end{pmatrix} \quad \text{and} \quad \mathbf{a}_2 = \frac{a_0}{2} \begin{pmatrix} 1 \\ \sqrt{3} \end{pmatrix}, \quad (\text{zig-zag convention}),$$

where $a_0 = \sqrt{3}d_0$ is the graphene lattice constant and d_0 is the distance between neighboring carbon atoms. For unit cell we take $\Gamma = [0, 1)\mathbf{a}_1 + [0, 1)\mathbf{a}_2$ as shown in Figure 4 and there are

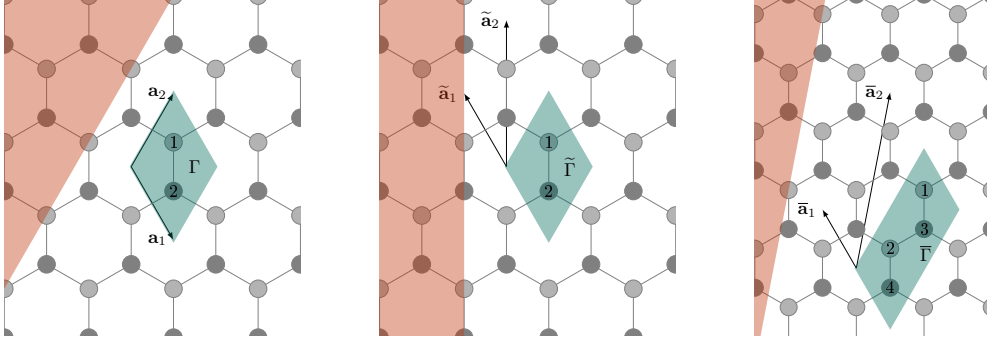


FIGURE 4. Our convention for the zigzag direction (left), armchair direction with $(n, m) = (-1, 1)$ (middle), and another angle with $(n, m) = (2, -1)$ (right). The shaded cell represents Γ (resp. $\tilde{\Gamma}$, $\bar{\Gamma}$).

$M = 2$ carbon atoms, located at $\mathbf{x}_1 = \frac{1}{3}(\mathbf{a}_1 + 2\mathbf{a}_2)$ and $\mathbf{x}_2 = \frac{1}{3}(2\mathbf{a}_1 + \mathbf{a}_2)$. The Wallace Hamiltonian only contains hopping between nearest neighbours, with

$$\begin{cases} (H\Psi)_{\mathbf{R}}^{(1)} &= t_0 \left(\Psi_{\mathbf{R}}^{(2)} + \Psi_{\mathbf{R}-\mathbf{a}_1}^{(2)} + \Psi_{\mathbf{R}+\mathbf{a}_2}^{(2)} \right), \\ (H\Psi)_{\mathbf{R}}^{(2)} &= t_0 \left(\Psi_{\mathbf{R}}^{(1)} + \Psi_{\mathbf{R}+\mathbf{a}_1}^{(1)} + \Psi_{\mathbf{R}-\mathbf{a}_2}^{(1)} \right). \end{cases}$$

Here, t_0 is the carbon-carbon hopping amplitude and since it just sets the energy scale, we will take $t_0 = 1$ throughout this Section. There are only five non-zero matrices $\mathbf{h}(\mathbf{R})$, given by

$$\mathbf{h}(\mathbf{0}) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \mathbf{h}(\mathbf{a}_1) = \mathbf{h}(-\mathbf{a}_2) = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad \mathbf{h}(-\mathbf{a}_1) = \mathbf{h}(\mathbf{a}_2) = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix},$$

We find that the Bloch fibers are given by

$$\mathbf{H}_{\mathbf{k}} = \begin{pmatrix} 0 & 1 + e^{-i\mathbf{k} \cdot \mathbf{a}_1} + e^{i\mathbf{k} \cdot \mathbf{a}_2} \\ c.c. & 0 \end{pmatrix}.$$

The map $\mathbf{k} \mapsto \mathbf{H}_{\mathbf{k}}$ is \mathbb{L}^* -periodic, with $\mathbb{L}^* = \mathbf{a}_1^* \mathbb{Z} \oplus \mathbf{a}_2^* \mathbb{Z}$, with

$$\mathbf{a}_1^* = \frac{2\pi}{\sqrt{3}a_0} \begin{pmatrix} \sqrt{3} \\ -1 \end{pmatrix}, \quad \mathbf{a}_2^* = \frac{2\pi}{\sqrt{3}a_0} \begin{pmatrix} \sqrt{3} \\ 1 \end{pmatrix}$$

The eigenvalues of $\mathbf{H}_{\mathbf{k}}$ are $\pm|1 + e^{-i\mathbf{k} \cdot \mathbf{a}_1} + e^{i\mathbf{k} \cdot \mathbf{a}_2}|$. Thus, the two bands are mirror images that meet at the so called Dirac points $\mathbf{k} \in \mathbf{K} + \mathbb{L}^*$ or $\mathbf{k} \in \mathbf{K}' + \mathbb{L}^*$, $\mathbf{K} := \frac{1}{3}(\mathbf{a}_1^* + \mathbf{a}_2^*)$ and $\mathbf{K}' := \frac{2}{3}(\mathbf{a}_1^* + \mathbf{a}_2^*)$. These are the only points where the gap closes.

4.3.2. Zigzag orientation. With this choice for the lattice vector \mathbf{a}_2 , and assuming as before that the wall is constant along the \mathbf{a}_2 -direction, we can see that the associated halfspace model would corresponds to the zig-zag or bearded cut (see the left panel of Fig. 4).

After a partial Fourier transform in the \mathbf{k}_2 direction, we find the Jacobi operator with blocks

$$b = h_{\mathbf{k}_2}(\mathbf{0}) = \begin{pmatrix} 0 & 1 + e^{-i\mathbf{k}_2 \cdot \mathbf{a}_2} \\ c.c. & 0 \end{pmatrix}, \quad a^* = h_{\mathbf{k}_2}(\mathbf{a}_1) = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}.$$

We recover the SSH matrices studied in Section 2.4, with $J_1 := 1 + e^{-i\mathbf{k}_2 \cdot \mathbf{a}_2}$ and $J_2 = 1$. Note that J_1 is now complex valued, but its phase can be removed by a unitary transformation that does not affect the wall potential.

For shortness, define $r(\mathbf{k}_2) = |1 + e^{-i\mathbf{k}_2 \cdot \mathbf{a}_2}| = |2 \sin(\frac{\mathbf{k}_2 \cdot \mathbf{a}_2}{2})|$. The essential spectrum is just

$$\sigma(H_{\mathbf{k}_2}) = \sigma_{\text{ess}}(H_{\mathbf{k}_2}) = [-|1 + r(\mathbf{k}_2)|, -|1 - r(\mathbf{k}_2)|] \cup [|1 - r(\mathbf{k}_2)|, |1 + r(\mathbf{k}_2)|],$$

The gap of the one-dimensional operator $H_{\mathbf{k}_2}$ closes only for $\mathbf{k}_2 = \frac{1}{3}\mathbf{a}_2^* + \mathbb{L}_2^*$ and $\mathbf{k}_2 = \frac{2}{3}\mathbf{a}_2^* + \mathbb{L}_2^*$, corresponding to the projections of the \mathbf{K} and \mathbf{K}' points on the line $\mathbf{a}_2^* \mathbb{R}$, along the \mathbf{a}_1^* -direction. This can be seen in the first panel of Figure 5. Apart from these two points, we have $\mathcal{N}_{\mathbf{k}_2}(E = 0) = 1$. Numerical simulations of the edge modes are presented in Figures 6 and 7.

Note that $r(\mathbf{k}_2) < 1$ if and only if $\mathbf{k}_2 \in (-1/3, 1/3)\mathbf{a}_2^*$ modulo \mathbb{L}_2^* . In some sense, the Dirac cones $\pm \frac{1}{3}\mathbf{a}_2^*$ separate the two phases $|J_1| < |J_2|$ and $|J_2| < |J_1|$ of the SSH model. According to Remark 2.6, this explains in particular why a hard cut would create a line of edge modes in the gap $(-1/3, 1/3)\mathbf{a}_2^*$ or in the gap $(1/3, 2/3)\mathbf{a}_2^*$ modulo \mathbb{L}_2^* , depending on the location of a hard wall with respect to the lattice, which corresponds either to a zigzag edge or to a bearded zigzag edge. Also note that the spectrum is symmetric around zero, and that for $\mathbf{k}_2 = \mathbf{a}_2/2$ (at the edge of the first Brillouin zone) the chain decouples and the essential spectrum is just $\{-1, 1\}$.

4.3.3. The armchair orientation. The armchair direction can be obtained by taking $n = -1$ and $m = 1$, that is (we use the tilde notation for the armchair convention) $\tilde{\mathbf{a}}_1 = -\mathbf{a}_1$, $\tilde{\mathbf{a}}_2 = -\mathbf{a}_1 + \mathbf{a}_2$, $\tilde{\mathbf{a}}_1^* = -\mathbf{a}_1^* - \mathbf{a}_2^*$ and $\tilde{\mathbf{a}}_2^* = \mathbf{a}_2^*$, namely

$$\tilde{\mathbf{a}}_1 = \frac{a_0}{2} \begin{pmatrix} -1 \\ \sqrt{3} \end{pmatrix}, \quad \tilde{\mathbf{a}}_2 = \frac{a_0}{2} \begin{pmatrix} 0 \\ 2\sqrt{3} \end{pmatrix}, \quad \tilde{\mathbf{a}}_1^* = \frac{2\pi}{\sqrt{3}a_0} \begin{pmatrix} -2\sqrt{3} \\ 0 \end{pmatrix}, \quad \tilde{\mathbf{a}}_2^* = \frac{2\pi}{\sqrt{3}a_0} \begin{pmatrix} \sqrt{3} \\ 1 \end{pmatrix}.$$

See Fig. 4 for the lattice configuration (middle) and Fig. 5 for the reciprocal space. The matrix elements are given by

$$\tilde{h}(\mathbf{0}) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \tilde{h}(\tilde{\mathbf{a}}_1) = \tilde{h}(\tilde{\mathbf{a}}_2 - \tilde{\mathbf{a}}_1) = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \quad \tilde{h}(-\tilde{\mathbf{a}}_1) = \tilde{h}(\tilde{\mathbf{a}}_1 - \tilde{\mathbf{a}}_2) = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}.$$

This time, the spectrum of $\tilde{H}_{\tilde{\mathbf{k}}_2}$ is the projection of the Bloch bands of the Wallace model along the horizontal direction, which sends the two inequivalent Dirac points \mathbf{K} and \mathbf{K}' into the single point $\mathbf{k}_2 = 0$. For all other values of $\tilde{\mathbf{k}}_2 \in \mathbb{R}\tilde{\mathbf{a}}_2^*$, there is a band gap, and $\mathcal{N}_{H_{\tilde{\mathbf{k}}_2}}(0) = 1$. So a spectral flow of -1 will appear when a wall is added and moved along $\tilde{\mathbf{a}}_1$.

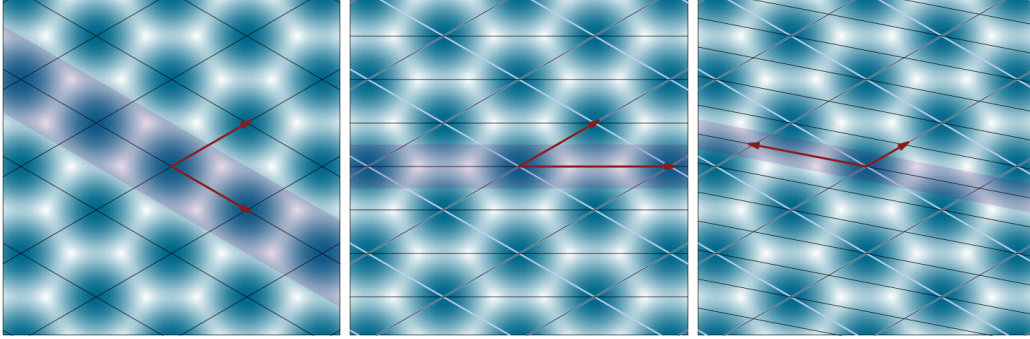


FIGURE 5. Brillouin zones and reciprocal vectors for the Wallace model corresponding to a zigzag cut, armchair cut ($n = 1, m = -1$) and a cut with $n = 2, m = -1$. In the second two pictures, the gray lines indicate the original Brillouin zone, which is covered by $|nm|$ copies of the new Brillouin zone. The blue-white gradient shows the upper energy band for the Wallace model, the white dots are the Dirac points. The band structure of $H_{\mathbf{k}_2}$ (resp. $\tilde{H}_{\tilde{\mathbf{k}}_2}$, $\overline{H}_{\overline{\mathbf{k}}_2}$) is obtained by projecting parallel to the shaded band onto the \mathbf{a}_2^* -vector (resp. $\tilde{\mathbf{a}}_2$, $\bar{\mathbf{a}}_2$) that points to the upper right corner.

4.3.4. Another rational cut. To illustrate the discussion in Section 4.2, we consider a different rational direction with $n = -1$ and $m = 2$, that is (we use the bar notation for this angle) $\bar{\mathbf{a}}_1 = -\mathbf{a}_1$, $\bar{\mathbf{a}}_2 = -\mathbf{a}_1 + 2\mathbf{a}_2$, $\bar{\mathbf{a}}_1^* = -\mathbf{a}_1^* - \frac{1}{2}\mathbf{a}_2^*$ and $\bar{\mathbf{a}}_2^* = \frac{1}{2}\mathbf{a}_2^*$, namely

$$\bar{\mathbf{a}}_1 = \frac{a_0}{2} \begin{pmatrix} -1 \\ \sqrt{3} \end{pmatrix}, \quad \bar{\mathbf{a}}_2 = \frac{a_0}{2} \begin{pmatrix} 1 \\ 3\sqrt{3} \end{pmatrix}, \quad \bar{\mathbf{a}}_1^* = \frac{\pi}{\sqrt{3}a_0} \begin{pmatrix} -3\sqrt{3} \\ 1 \end{pmatrix}, \quad \bar{\mathbf{a}}_2^* = \frac{\pi}{\sqrt{3}a_0} \begin{pmatrix} \sqrt{3} \\ 1 \end{pmatrix}.$$

The lattice structure is shown in the rightmost panel of Figure 4 and the reciprocal lattice in Figure 5. This time, the lattice $\bar{\mathbb{L}} := \bar{\mathbf{a}}_1\mathbb{Z} \oplus \bar{\mathbf{a}}_2\mathbb{Z}$ strictly contains the initial graphene lattice \mathbb{L} . The corresponding new unit cell $\tilde{\Gamma}$ consists of two copies of the original unit cell and contains 4

atoms. In order to construct the 4×4 matrices that will give \mathbf{h} , it is convenient to label first the sites on one sublattice and then those on the other sublattice, so that \mathbf{h} is block-off-diagonal, see again Fig. 4.

This gives $\bar{\mathbf{h}}(\mathbf{R}) = \begin{pmatrix} 0 & f(\mathbf{R}) \\ g(\mathbf{R}) & 0 \end{pmatrix}$ with $g(\mathbf{R}) = f(-\mathbf{R})^*$. The nonzero entries are given by

$$f(\mathbf{0}) = \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix}, \quad f(-\bar{\mathbf{a}}_1) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad f(\bar{\mathbf{a}}_1 - \bar{\mathbf{a}}_2) = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

and $f(\bar{\mathbf{R}}) = 0$ otherwise. The operator $\bar{H}_{\mathbf{k}_2}$ is defined for $\mathbf{k}_2 \in \mathbb{R}\bar{\mathbf{a}}_2^*$, and is $\bar{\mathbf{a}}_2^*$ -periodic. Note that $|\bar{\mathbf{a}}_2^*| = \frac{1}{2}|\mathbf{a}_2^*|$: the Brillouin zone is twice smaller than in the previous cases. Simple geometric considerations shows that \mathbf{K} and \mathbf{K}' Dirac point are projected on $\pm \frac{1}{3}\bar{\mathbf{a}}_2^*$ modulo $\bar{\mathbf{a}}_2^*\mathbb{Z}$. Note that the two projections differ. In the terminology of [1, 9], this angle is of *zig-zag* type. It is of *armchair* type if the projections of \mathbf{K} and \mathbf{K}' coincide. In our work however, there are no fundamental differences between these two cases. Except from these special values, there is a gap around zero, but now $\mathcal{N}_{H_{\bar{\mathbf{k}}_2}}(0) = 2$, so a spectral flow of -2 appears in the gap.

4.3.5. Numerical illustration of the edge spectrum for different cuts. For the three cuts described before, we numerically compute the corresponding edge (and bulk) spectra¹. We use the same strategy as in Section 2.4 to detect edge modes.

For the soft wall, we took $w_t(\mathbf{x})$ of the form (21)-(22), with the scalar potential

$$v_1(x) := \begin{cases} 0 & \text{for } x \geq 0 \\ -\nu x & \text{for } x \leq 0. \end{cases}$$

The corresponding edge models $H^\sharp(t)$ (zigzag orientation), $\tilde{H}^\sharp(t)$ (armchair orientation) and $\bar{H}^\sharp(t)$ (our commensurate angle with $n = 2$ and $m = -1$, called *angle* in what follows) are 1-quasi-periodic. Recall that our results shows that, outside the projection of the Dirac cones, we must have

$$\text{Sf}\left(H_{\mathbf{k}_2}^\sharp(t), [0, 1], E\right) = \text{Sf}\left(\tilde{H}_{\bar{\mathbf{k}}_2}^\sharp(t), [0, 1], E\right) = 1 \quad \text{while} \quad \text{Sf}\left(\bar{H}_{\bar{\mathbf{k}}_2}^\sharp(t), [0, 1], E\right) = 2. \quad (25)$$

The edge modes as functions of k_2 . In Figure 7, we plot the edge spectra of $\mathbf{k}_2 \mapsto H_{\mathbf{k}_2}(t)$, $\tilde{\mathbf{k}}_2 \mapsto \tilde{H}_{\tilde{\mathbf{k}}_2}(t)$ and $\bar{\mathbf{k}}_2 \mapsto \bar{H}_{\bar{\mathbf{k}}_2}(t)$ for different values of $t \in [0, 1]$, and with the Lipschitz constant $\nu = 1$. The grey parts represent the bulk essential spectrum, and the red curves are the edge eigenvalues.

In these plots, the x -axis corresponds to $|\mathbf{k}_2|$, respectively $|\tilde{\mathbf{k}}_2|$, $|\bar{\mathbf{k}}_2|$. By periodicity, we represent the plots on a portion $[-\frac{1}{2}|\mathbf{a}_2^*|, \frac{1}{2}|\mathbf{a}_2^*|]$, etc. Note that $|\bar{\mathbf{a}}_2^*| = \frac{1}{2}|\tilde{\mathbf{a}}_2^*| = \frac{1}{2}|\mathbf{a}_2^*|$, so the x -axis for the last plot is twice smaller.

According to these simulations, it seems that the edge mode curves $\mathbf{k}_2 \mapsto \lambda(\mathbf{k}_2)$ do not necessarily starts and ends at the Dirac cones, as is probably the case for hard cut truncations [9]. One reason is that the addition of a soft wall breaks the chiral symmetry: the spectrum of $H^\sharp(t)$ is no longer symmetric with respect to the origin, so the eigenvalue $E = 0$ no longer plays a special role for edge modes.

Another remark is that there is no qualitative difference between the different cuts: we see edge curves in each gap.

The edge modes as functions of t . In Figure 7, we fix $\mathbf{k}_2 = \frac{1}{6}\mathbf{a}_2^*$, $\tilde{\mathbf{k}}_2 = \frac{1}{6}\tilde{\mathbf{a}}_2^*$ and $\bar{\mathbf{k}}_2 = \frac{1}{6}\bar{\mathbf{a}}_2^*$, and plot the edge spectra of $t \mapsto H_{\mathbf{k}_2}(t)$, $t \mapsto \tilde{H}_{\tilde{\mathbf{k}}_2}(t)$ and $t \mapsto \bar{H}_{\bar{\mathbf{k}}_2}(t)$. We took different values of the Lipschitz constants. In these figures, we clearly observe the expected spectral flows in (25), and that the curves become steeper and steeper as ν increases.

¹The code can be found here: https://gitlab.com/davidgontier/softwall_jacobimatrix

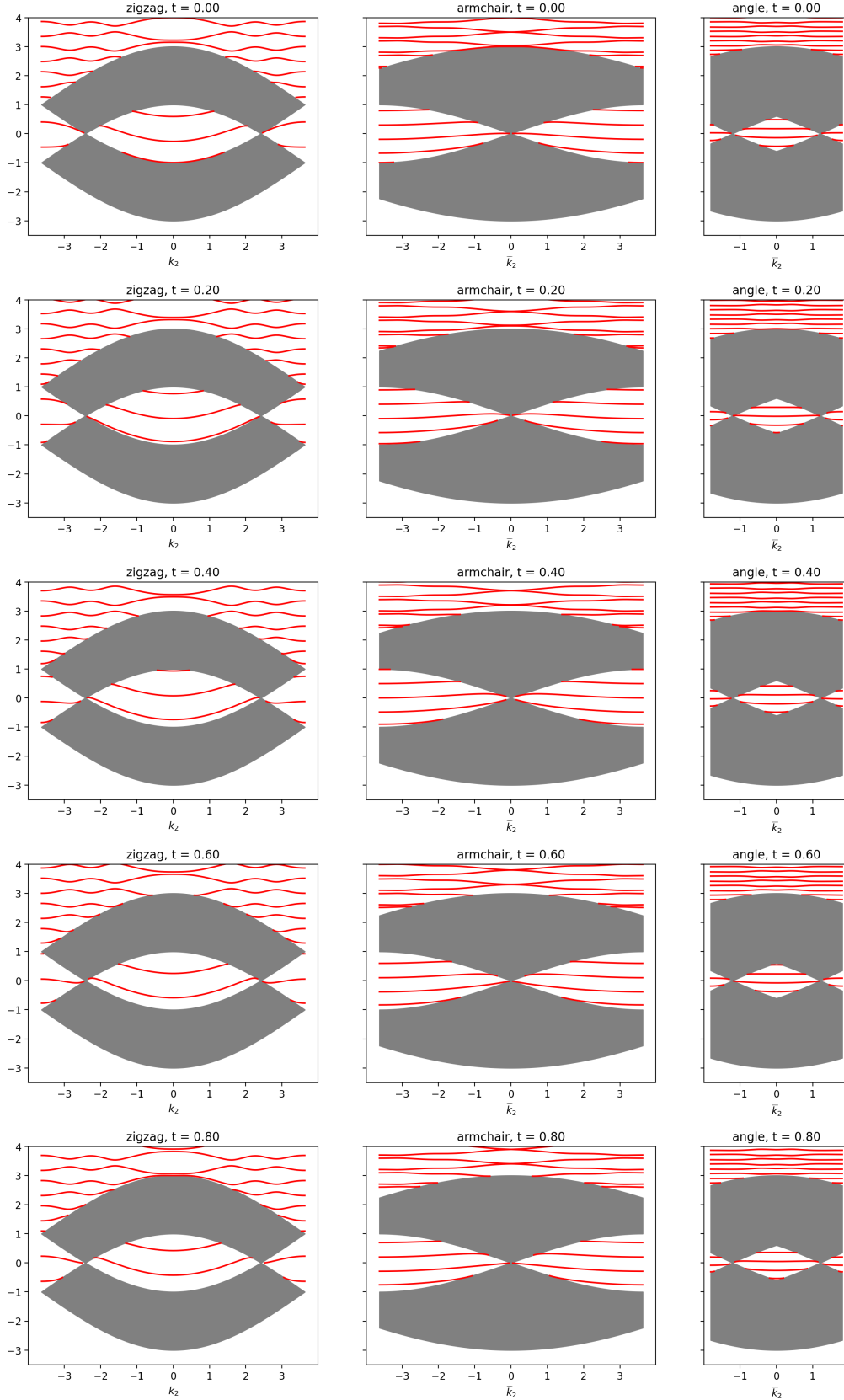


FIGURE 6. Spectrum of the edge Hamiltonians $\mathbf{k}_2 \mapsto H_{\mathbf{k}_2}^\sharp(t)$, $\tilde{\mathbf{k}}_2 \mapsto \tilde{H}_{\tilde{\mathbf{k}}_2}^\sharp(t)$ and $\bar{\mathbf{k}}_2 \mapsto \bar{H}_{\bar{\mathbf{k}}_2}^\sharp(t)$ for different values of $t \in \{0, 0.2, 0.4, 0.6, 0.8\}$, and with $\nu = 1$.

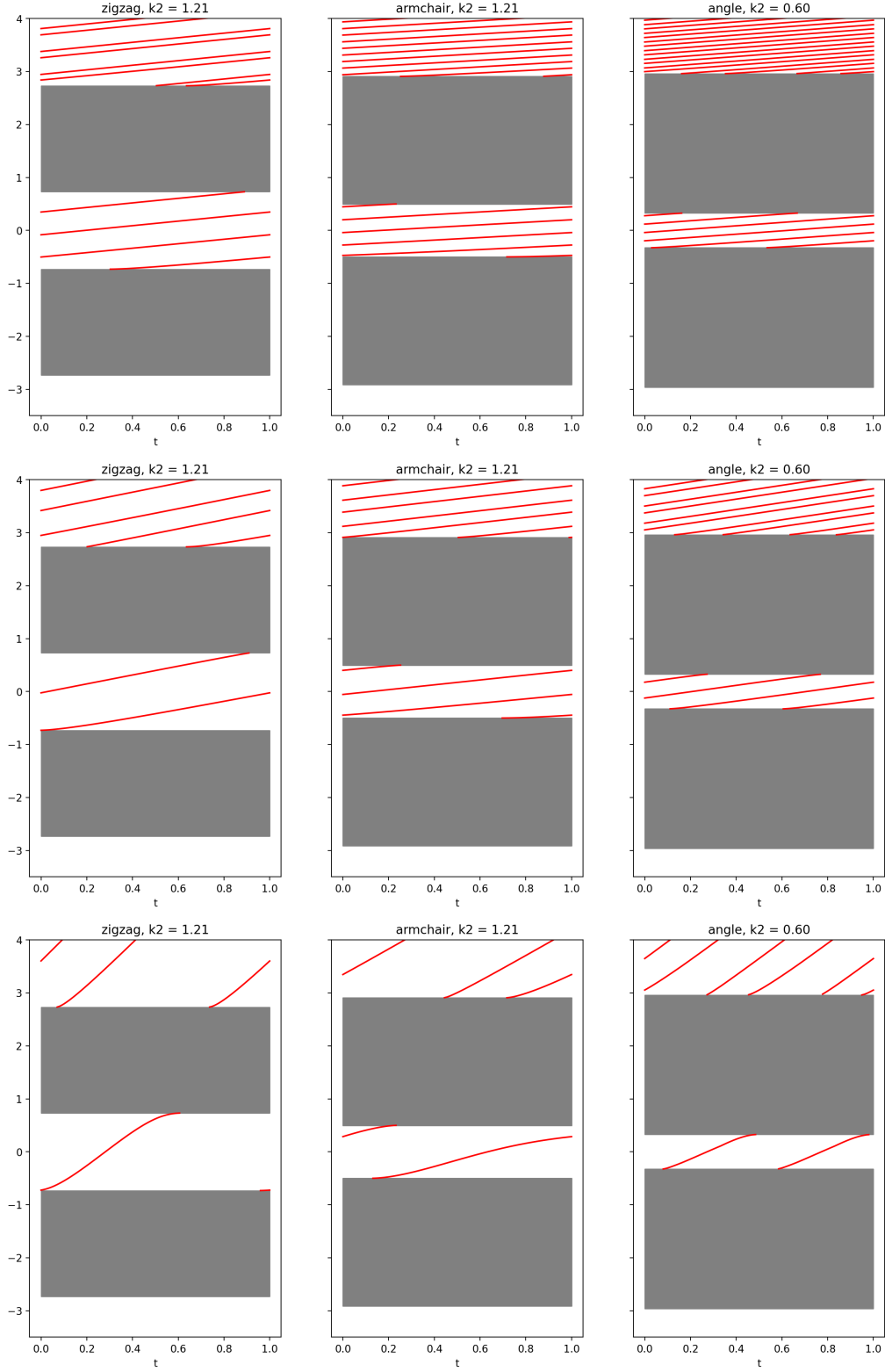


FIGURE 7. Spectrum of the edge Hamiltonians $t \mapsto H_{\mathbf{k}_2}(t)$, $t \mapsto \tilde{H}_{\mathbf{k}_2}(t)$ and $t \mapsto \bar{H}_{\mathbf{k}_2}(t)$ for different values of $\nu \in \{0.5, 1, 5\}$.

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APPENDIX A. THE SPECTRAL FLOW

The notion of spectral flow has been introduced in [2, 3], and studied extensively in the case of continuous path of symmetric Fredholm operators (see also [27] and the recent book [8] for a complete picture). Recall that for a bounded self-adjoint operator A , the operator $A - E$ is Fredholm iff E is not in the essential spectrum of A . In the unbounded case, we can work instead with the family $B_t := f(A_t - E)$, where f is a bounded increasing function with $f(\lambda) = \lambda$ around $\lambda = 0$. The goal of this Appendix is to give a self-contained version of the Spectral flow, using only tools from spectral theory, and which is enough for our purpose.

A.1. Norm resolvent topology. In what follows, we fix \mathcal{H} a separable Hilbert space. We define the norm-resolvent metric on the set of (possibly unbounded) self-adjoint operators $\mathcal{A}(\mathcal{H})$ acting on \mathcal{H} by

$$d(A, B) := \|\mathcal{R}(i, A) - \mathcal{R}(i, B)\|_{\text{op}},$$

where we set $\mathcal{R}(z, A) := (z - A)^{-1}$. This endows $\mathcal{A}(\mathcal{H})$ with the norm-resolvent topology. Recall that the point $i \in \mathbb{C}$ does not play any special role, and that, for all $z \in \mathbb{C} \setminus \mathbb{R}$, the corresponding metric with z instead of i defines the same topology. More specifically, if $d_z(A, B) := \|(z - A)^{-1} - (z - B)^{-1}\|_{\text{op}}$, we have the following.

Lemma A.1. *Let A be a self-adjoint operator, and let $z \in \mathbb{C} \setminus \sigma(A)$. Then there is $\varepsilon > 0$ and $C \geq 0$ so that, for all self-adjoint operators B with $d(A, B) < \varepsilon$, we have $z \in \mathbb{C} \setminus \sigma(B)$, and $\|(z - B)^{-1} - (z - A)^{-1}\|_{\text{op}} \leq Cd(A, B)$.*

Proof. We follow [23, Remark IV.3.13]. For $z, z_0 \in \mathbb{C}$, we formally have

$$\mathcal{R}(z, A) - \mathcal{R}(z, B) = \frac{z_0 - A}{z - A} [\mathcal{R}(z_0, A) - \mathcal{R}(z_0, B)] \frac{z_0 - B}{z - B}.$$

In addition, since $\frac{z - B}{z_0 - B} = 1 + (z - z_0)\mathcal{R}(z_0, B)$ and, similarly, $\frac{z - A}{z_0 - A} = 1 + (z - z_0)\mathcal{R}(z_0, A)$, we deduce that

$$\begin{aligned} \frac{z - B}{z_0 - B} &= \frac{z - A}{z_0 - A} + (z - z_0) [\mathcal{R}(z_0, B) - \mathcal{R}(z_0, A)] \\ &= \frac{z - A}{z_0 - A} \left[1 + (z - z_0) \frac{z_0 - A}{z - A} [\mathcal{R}(z_0, B) - \mathcal{R}(z_0, A)] \right]. \end{aligned}$$

In particular, if $(z_0 - A)$ and $(z - A)$ are invertible with bounded inverse, and if $\|\mathcal{R}(z_0, B) - \mathcal{R}(z_0, A)\|_{\text{op}}$ is sufficiently small, then we deduce that $(z - B)$ is also invertible. Actually,

$$\mathcal{R}(z, A) - \mathcal{R}(z, B) = \frac{z_0 - A}{z - A} [\mathcal{R}(z_0, A) - \mathcal{R}(z_0, B)] \left[1 + (z - z_0) \frac{z_0 - A}{z - A} [\mathcal{R}(z_0, B) - \mathcal{R}(z_0, A)] \right]^{-1} \frac{z_0 - B}{z - B}.$$

In particular, with $z_0 = i$,

$$d_z(A, B) \leq \frac{\left\| \frac{i - A}{z - A} \right\|_{\text{op}}^2 d(A, B)}{1 - |z - i| \left\| \frac{i - A}{z - A} \right\|_{\text{op}} d(A, B)},$$

which makes sense whenever $d(A, B) < \left(|z - i| \left\| \frac{i - A}{z - A} \right\|_{\text{op}} \right)^{-1}$. □

Lemma A.2. *If A is self-adjoint and H is bounded self-adjoint, then the map $\lambda \mapsto A + \lambda H$ is continuous for the norm-resolvent metric. In particular $\mathbb{R} \ni \lambda \mapsto A - \lambda$ is continuous.*

Proof. Let us prove continuity at $\lambda_0 \in \mathbb{R}$. We have

$$\frac{1}{i - (A + \lambda H)} - \frac{1}{i - (A + \lambda_0 H)} = (\lambda - \lambda_0) \frac{1}{i - (A + \lambda H)} H \frac{1}{i - (A + \lambda_0 H)}.$$

Since A and $A + \lambda H$ are self-adjoint, we have $\|(i - A)^{-1}\|_{\text{op}} \leq 1$ (and similarly for $A + \lambda H$), so $d(A + \lambda_0 H, A + \lambda H) \leq |\lambda - \lambda_0| \cdot \|H\|_{\text{op}}$, which implies continuity. \square

A.2. Definition of the Spectral Flow. We consider a family $[0, 1] \ni t \mapsto A_t$ of self-adjoint operators on \mathcal{H} , continuous for this topology. We denote by $\sigma(\{A_t\})$ and $\sigma_{\text{ess}}(\{A_t\})$ the spectrum and essential spectrum of the family $\{A_t\}$ as the closure of the union (over t) of the spectra and essential spectra. Namely,

$$\sigma(\{A_t\}) := \overline{\bigcup_{t \in [0, 1]} \sigma(A_t)} \quad \text{and} \quad \sigma_{\text{ess}}(\{A_t\}) := \overline{\bigcup_{t \in [0, 1]} \sigma_{\text{ess}}(A_t)}.$$

Both $\sigma(\{A_t\})$ and $\sigma_{\text{ess}}(\{A_t\})$ are closed subsets of \mathbb{R} . Our goal is to define the spectral flow $\text{Sf}(A_t, E, t \in [0, 1])$ for any $E \in \mathbb{R} \setminus \sigma_{\text{ess}}(\{A_t\})$. It will correspond to the net number of branches of eigenvalues of A_t crossing the energy E downwards.

Recall that for any self-adjoint operator A , if $(E - g, E + g) \cap \sigma_{\text{ess}}(A) = \emptyset$, then there is $0 \leq a \leq g$ so that both numbers $E - a$ and $E + a$ are not in the spectrum of A (if $E \notin \sigma(A)$, one can simply take $a = 0$). The spectral projector $P_{(E-a, E+a)}(A)$ is then of finite rank, and given by the Cauchy integral

$$P_{(E-a, E+a)}(A) = P_{[E-a, E+a]}(A) = \frac{1}{2i\pi} \oint_{\mathcal{C}} \frac{dz}{z - A},$$

where \mathcal{C} is the positively oriented complex circle of center E and radius a . We recall the following classical result. We skip the proof.

Lemma A.3. *With the same notation as before, there is $\varepsilon > 0$ so that the map $B \mapsto P_{(E-a, E+a)}(B)$ is continuous on $\{B \in \mathcal{A}(\mathcal{H}), d(A, B) < \varepsilon\}$. In particular, we have $\text{rank } P_{(E-a, E+a)}(B) = \text{rank } P_{(E-a, E+a)}(A)$ for all such B .*

We can now define the spectral flow of $\{A_t\}$ at the energy E . For all $t \in [0, 1]$, we let $a(t) \geq 0$ be so that $\{E \pm a(t)\}$ are not in the spectrum of A_t . By Lemma A.3, there is $\varepsilon(t) > 0$ so that the result of the Lemma holds. Set

$$U(t) := \{t' \in [0, 1], \quad d(A_t, A_{t'}) < \varepsilon(t)\}.$$

By continuity of the map $t \mapsto A_t$, the set $U(t)$ is an open set of $[0, 1]$, and the union of all $U(t)$ covers the compact set $[0, 1]$. By classical arguments, we can find a subdivision $0 = t_0 < t_1 < \dots < t_M = 1$ and real non-negative numbers $a_1, a_2, \dots, a_M \geq 0$, which we call the *widths*, so that

$$\forall 1 \leq i \leq M, \quad [t_{i-1}, t_i] \ni t \mapsto P_{(E-a_i, E+a_i)}(A_t) \quad \text{is continuous on } [t_{i-1}, t_i]. \quad (26)$$

In other words, the spectrum of A_t does not cross the levels $\{E \pm a_i\}$ for $t \in [t_{i-1}, t_i]$. Notice in particular that $E + a_i$ and $E + a_{i+1}$ do not belong to the spectrum of A_i . The **spectral flow** of $\{A_t\}$ is defined by

$$\text{Sf}(A_t, E, t \in [0, 1]) := \sum_{i=1}^M \text{rank } P_{(E, E+a_i)}(A_{t_{i-1}}) - \text{rank } P_{(E, E+a_i)}(A_{t_i}).$$

Note that E may be an eigenvalue of A_{t_i} here, so that $P_{(E, E+a_i)}$ is the spectral projection of A_{t_i} , including the eigenspace $\text{Ker}(A_i - E)$. It is unclear with this definition that the spectral flow has nice topological properties. However, after relabelling the sums, we get the equivalent formula

$$\boxed{\text{Sf}(A_t, E, t \in [0, 1]) = \dim \text{Ker}(A_0 - E) - \dim \text{Ker}(A_1 - E) + \sum_{i=1}^{M-1} \text{rank } P_{(E+a_i, E+a_{i+1})}(A_{t_i}),} \quad (27)$$

with the convention that $\text{rank } P_{(a,b)}(A) = -\text{rank } P_{(b,a)}(A)$ if $b < a$. Note that due to the boundary terms, the spectral flows depends on the value of E in the gap. However, if we restrict the spectral

flow to operators A_t satisfying $\dim \text{Ker}(A_0 - E) = \dim \text{Ker}(A_1 - E)$, then we will prove below that the spectral flow is independent of E in the gap. This happens in particular if A_1 is unitarily equivalent to A_0 .

It is a classical result (see [27]) that the spectral flow is a well-defined quantity, which is independent of the choice of the (t_i) and the (a_i) . The only condition is that the family (t_i, a_i) satisfies (26). The following example illustrates that the spectral flow counts the number of branches of eigenvalue going downwards.

Example A.1. Assume that the spectrum of A_t exhibits a single decreasing branch of eigenvalue $\lambda(t)$ crossing downwards the energy E at $t_* \in (0, 1)$. For the subdivision, take $M = 3$, $t_0 = 1$, $t_1 = t_* - \varepsilon$, $t_2 = t_* + \varepsilon$ and $t_3 = 1$, and set $a_1 = 0$, $a_2 = a > 0$, $a_3 = 0$, where $a > \max\{\lambda(t_1) - \lambda(t_*), \lambda(t_*) - \lambda(t_2)\}$. Then we get

$$\text{rank } P_{(E+a_1, E+a_2)}(A_{t_1}) = 1, \quad \text{rank } P_{(E+a_2, E+a_3)}(A_{t_2}) = 0,$$

so the spectral flow equals 1 in this case. See also Fig. 8.

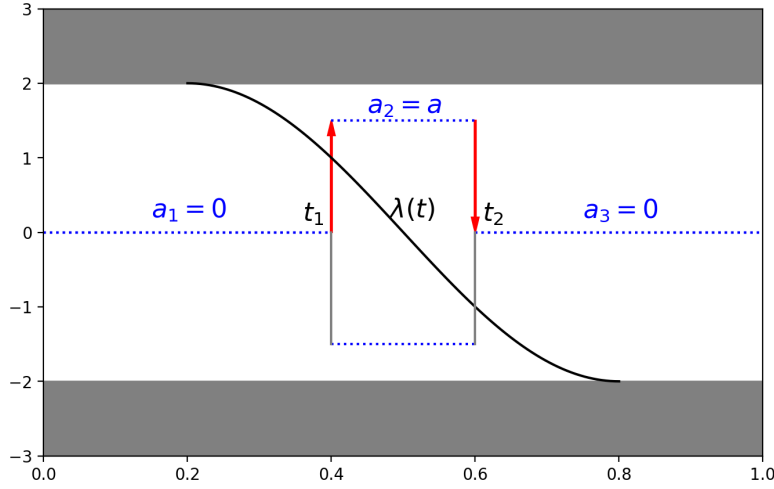


FIGURE 8. The subdivision (t_i) and corresponding widths (a_i) . In this example, the spectral flow is 1 at $E = 0$. The spectral flow is a signed sum of branches of eigenvalues crossing the red horizontal segments (sign + if the arrow is upwards, sign - otherwise).

A.3. Stability of the spectral flow. The Spectral flow is stable in the following sense.

Lemma A.4. Let A_t be a continuous operator family and $E \in \mathbb{R} \setminus \sigma_{\text{ess}}(\{A_t\})$. There is $\varepsilon > 0$ so that, for any norm-resolvent continuous family (B_t) of self-adjoint operators satisfying $d(A_t, B_t) < \varepsilon$ for all $t \in [0, 1]$ and $B_0 = A_0$, $B_1 = A_1$, it holds $\text{Sf}(A_t, E, [0, 1]) = \text{Sf}(B_t, E, [0, 1])$.

We emphasize that we require that the paths (A_t) and (B_t) have the same endpoints here. This is due to the boundary terms in (27).

Proof. Let $\{t_i\}$ be a subdivision for $\{A_t\}$, and $a_i \geq 0$ the corresponding widths, so that (26) holds. Let us fix $1 \leq i \leq M$. For all $t \in [t_{i-1}, t_i]$, we apply Lemma A.3, and find $\varepsilon(t) > 0$ so that the spectral projector on $(E - a_i, E + a_i)$ is continuous on $\{B, d(A_t, B) < \varepsilon(t)\}$. We set

$$U(t) := \left\{ t' \in [t_{i-1}, t_i], d(A_t, A_{t'}) < \frac{1}{2} \varepsilon(t) \right\}.$$

The open sets $U(t)$ cover the compact interval $[t_{i-1}, t_i]$, so we can find a sub-division $t_{i-1} = t_i^{(1)} < t_i^{(2)} < \dots < t_i^{(N_i)} = t_i$ so that the union of $\left(U(t_i^{(j)}) \right)_{1 \leq j \leq N_i}$ covers $[t_{i-1}, t_i]$.

We set $\varepsilon_i := \frac{1}{2} \min_j \{\varepsilon(t_i^{(j)})\}$. Now, assume that (B_t) is such that $d(A_t, B_t) < \varepsilon_i$ for all $t \in [t_{i-1}, t_i]$. Then, for such a t , let $1 \leq j \leq N_i$ be such that $t \in U(t_i^{(j)})$, and we have

$$d(A_{t_i^{(j)}}, B_t) < d(A_{t_i^{(j)}}, A_t) + d(A_t, B_t) \leq \frac{1}{2} \varepsilon(t_i^{(j)}) + \varepsilon_i < \varepsilon(t_i^{(j)}).$$

This shows that $P_{(E-a_i, E+a_i)}(B_t)$ is well-defined, with

$$\text{rank } P_{(E-a_i, E+a_i)}(B_t) = \text{rank } P_{(E-a_i, E+a_i)}(A_t).$$

In order to gather all the intervals $[t_{i-1}, t_i]$, we set $\varepsilon := \min_i \varepsilon_i$. For a family (B_t) with $d(A_t, B_t) < \varepsilon$, we deduce that the subdivision (t_i) with widths (a_i) is a valid one for (B_t) . In particular, we find that $E + a_i$ and $E + a_{i+1}$ are in the resolvent set for all choices of B_{t_i} with $d(A_{t_i}, B_{t_i}) < \varepsilon$, and hence

$$\text{rank } P_{(E+a_i, E+a_{i+1})}(B_{t_i}) = \text{rank } P_{(E+a_i, E+a_{i+1})}(A_{t_i}).$$

Since we also have $B_0 = A_0$ and $B_1 = A_1$, we obtain $\text{Sf}(A_t, E, [0, 1]) = \text{Sf}(B_t, E, [0, 1])$. \square

Lemma A.5. *Let $(s, t) \mapsto (A_t^{(s)})$ be a norm-resolvent continuous family of self-adjoint operators, such that the endpoints $A_0^{(s)} = A_0$ and $A_1^{(s)} = A_1$ are independent of s . Assume in addition that $\text{Sf}(A_t^{(s)}, E, t \in [0, 1])$ is well-defined for all s . Then this spectral flow is independent of s .*

This result follows by taking a suitable subdivision in the homotopy parameter s and applying the previous Lemma. The bottomline is that the only obstruction for homotopic invariance is that the spectral flow at E becomes ill-defined, which happens when the essential gap closes.

Recall the Weyl's theorem, which states that if A is self-adjoint and K is compact symmetric, then $A + sK$ is self-adjoint, and $\sigma_{\text{ess}}(A + sK) = \sigma(A)$ for all s : the essential gaps are stable under compact perturbations, and therefore never close. Applying the previous lemma to $A_t^{(s)} := A_t + sK$ gives the following result.

Lemma A.6. *Let (K_t) be a continuous family of symmetric compact operators with $K_0 = K_1 = 0$. Then $\text{Sf}(A_t, E, [0, 1]) = \text{Sf}(A_t + K_t, E, [0, 1])$.*

There is no assumption on the smallness of the family (K_t) in the compact case. Finally, we record the following useful result.

Lemma A.7. *If $f : \mathbb{R} \rightarrow \mathbb{R}$ is a strictly increasing function, then*

$$\text{Sf}(f(A_t), f(E), [0, 1]) = \text{Sf}(A_t, E, [0, 1]).$$

Here, $f(A_t)$ is defined via the spectral calculus. We skip the proof, as it is straightforward. In the case where (A_t) are uniformly bounded from below by some C , one can take $f_1(x) := (C - x)^{-1}$ and $f_2(x) = x - (C - E)^{-1}$, and deduce that

$$\text{Sf}(A_t, E, [0, 1]) = \text{Sf}((C - A_t)^{-1}, (C - E)^{-1}, [0, 1]) = \text{Sf}((C - A_t)^{-1} - (C - E)^{-1}, 0, [0, 1])$$

The advantage of the right-hand side is that the family $t \mapsto (C - A_t)^{-1} - (C - E)^{-1}$ is a norm continuous family of **bounded** symmetric operators, for which 0 is not in the essential spectrum. So this family is Fredholm self-adjoint, and we are back to the *usual* theory.

A.4. The spectrum quasi-periodic case. In the previous section, the spectral flow depends on the energy E in the gap. This is due to the presence of boundary terms in (27).

For $I \subset \mathbb{R}$ an interval of \mathbb{R} , we denote by \mathcal{C}_I the set of norm-resolvent continuous paths of self-adjoint operator (A_t) satisfying that

$$\forall E \in I, \quad \dim \text{Ker}(A_0 - E) = \dim \text{Ker}(A_1 - E).$$

Typical examples are:

- If $\mathbb{R} \ni t \mapsto (A_t)$ is 1-periodic in t , that is $A_{t+1} = A_t$, then (A_t) is in \mathcal{C}_I with $I = \mathbb{R}$.
- If A_1 is unitary equivalent to A_0 , say $A_1 = U A_0 U^*$, then (A_t) is in \mathcal{C}_I with $I = \mathbb{R}$.
- If $A_1 = \Sigma \oplus A_0$ (as in Section 3.2), then (A_t) is in \mathcal{C}_I with $I = (-\infty, \Sigma)$ or $I = (\Sigma, +\infty)$.

In this case, the boundary terms in (27) cancels, and we obtain the simpler formula

$$\boxed{\text{Sf}(A_t, E, t \in [0, 1]) = \sum_{i=1}^{M-1} \text{rank } P_{(E+a_i, E+a_{i+1})}(A_{t_i})} \quad \text{for } A \in \mathcal{C}_I, \quad \text{and } E \in I.$$

Now, the results of the previous Lemma holds, without the endpoints constraint. Mimicking the proof of Lemma A.4 gives the following.

Lemma A.8. *Let A_t be a continuous operator family in \mathcal{C}_I , and let $E \in I \setminus \sigma_{\text{ess}}(\{A_t\})$. There is $\varepsilon > 0$ so that, for any norm-resolvent continuous family (B_t) of self-adjoint operators satisfying $d(A_t, B_t) < \varepsilon$ for all $t \in [0, 1]$ and such that $A_t + B_t \in \mathcal{C}_I$, we have $\text{Sf}(A_t, E, [0, 1]) = \text{Sf}(B_t, E, [0, 1])$.*

From this stability Lemma, we easily deduce the counterpart of Lemma A.5.

Lemma A.9. *Let $(s, t) \mapsto (A_t^{(s)})$ be a norm-resolvent continuous family of self-adjoint operators, such that, for all s , the family $t \mapsto A_t^{(s)}$ is in \mathcal{C}_I . Let $E \in I$, and assume that $\text{Sf}(A_t^{(s)}, E, t \in [0, 1])$ is well-defined for all s . Then this spectral flow is independent of s .*

In particular, using Lemma A.2 stating that $\lambda \mapsto A - \lambda$ is continuous, we get the following.

Lemma A.10. *Let $(A_t) \in \mathcal{C}_I$, and let $g \subset \mathbb{R} \setminus \sigma_{\text{ess}}(\{A_t\})$ be an essential gap of the family (A_t) , so that $g \subset I$. Then the spectral flow $\text{Sf}(A_t, E, [0, A])$ is independent of E in the gap g .*

Finally, we state the counterpart of Lemma A.6.

Lemma A.11. *Let (K_t) be a continuous family of symmetric compact operators such that, for all $s \in [0, 1]$, we have $(A_t + sK_t) \in \mathcal{C}_I$. Then, for $E \in I$, we have $\text{Sf}(A_t, E, [0, 1]) = \text{Sf}(A_t + K_t, E, [0, 1])$.*

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