J. Spectr. Theory 12 (2022), 1155–1202
DOI 10.4171/JST/430

Edge states for second order elliptic operators in a channel

David Gontier

Abstract. We present a general framework to study edge states for second order elliptic operators in a half channel. We associate an integer valued index to some bulk materials, and we prove that, for any junction between two such materials, localized states must appear at the boundary whenever the indices differ.

1. Introduction and statement of the main results

Bulk-edge correspondence states that one can associate an integer valued index $\mathcal{I} \in \mathbb{Z}$ to some bulk materials (represented here by Schrödinger (PDE) or Hill's (ODE) operators). When the material is cut, edge states appear at the boundary whenever $\mathcal{I} \neq 0$. In addition, it is believed that any junction between a left and a right material having indices $\mathcal{I}_L$ and $\mathcal{I}_R$ must also have edge states near the junction whenever $\mathcal{I}_L \neq \mathcal{I}_R$. We prove this fact in this paper.

Since the original works of Hatsugai [24, 25], most studies on bulk-edge correspondence focused on tight-binding models (e.g., [3, 22]), set on half-spaces. In these tight-binding models, boundary conditions at the cut are quite simple to describe, and it turns out that the index is independent of these boundary conditions. In the context of continuous models, it is unclear that one can define an index which is indeed independent of the chosen boundary conditions. In [20], we proved that it was the case in a simple one-dimensional model for dislocations. We extend this work here, and give a general framework to define the edge index for different self-adjoint extensions of Schrödinger operators.

We consider two types of continuous models. In the first part, we study families of Hill's operator (ODE) set on $\mathbb{C}^n$, of the form

$$h_t := -\partial_{xx}^2 + V_t(x), \quad \text{acting on } L^2(\mathbb{R}, \mathbb{C}^n),$$

where $t \mapsto V_t$ is a continuous periodic family of bounded potentials, with values in the set of $n \times n$ hermitian matrices. When t is seen as the time variable, this equation

2020 Mathematics Subject Classification. Primary 35P05; Secondary 58J30.
Keywords. Dislocations, charge pumping, spectral flow, Lagrangian planes, Maslov index.

models a Thouless pump [9, 42]. In the case where $V_t(x) = V(x-t)$, the variable t is interpreted as a dislocation parameter [16, 20]. On the second part of the article, we study its PDE version, that is families of Schrödinger's operators of the form

$$H_t := -\Delta + V_t(x, y), \quad \text{acting on } L^2(\mathbb{R} \times (0,1)^{d-1}, \mathbb{C}).$$

Here, $\mathbb{R} \times (0,1)^{d-1}$ is a tube in $\mathbb{R}^d$, and we impose periodic boundary conditions in the last $(d-1)$-directions. Our setting also allows to treat two-dimensional PDE operators of the form

$$\widetilde{H_t} := -\partial_{xx}^2 + (-\mathrm{i}\partial_y + 2\pi t)^2 + V(x, y), \quad \text{acting on } L^2(\mathbb{R} \times (0,1), \mathbb{C}),$$

where $k := 2\pi t$ is interpreted as the Bloch quasi-momentum in the y-direction. Such families of operators appear in the study of two-dimensional materials, once a Bloch transform has been performed in the y-direction.

In these models, we interpret the bulk-edge index as the intersection of Lagrangian planes on a *boundary space* $\mathcal{H}_b$. Roughly speaking, this space contains the values $(\psi(0), \psi'(0))$ of the admissible wave-functions ψ. In the context of Hill's operators, we take $\mathcal{H}_b = \mathbb{C}^n \times \mathbb{C}^n$, while for Schrödinger operators, $\mathcal{H}_b = H^{3/2}(\Gamma) \times H^{1/2}(\Gamma)$, where $\Gamma := \{0\} \times (0,1)^{d-1}$ is the cut.

The link between edge states and Lagrangian planes was already mentioned, e.g., in [3] for discrete models (tight-binding approximation). Based on the recent developments on Lagrangian planes and second order elliptic operator by Howard, Latushkin and Sukhtayev in a series on papers [28–30] (see [32] for older results in an ODE setting), we extend the picture to the continuous case. This framework allows in particular to treat the PDE setting following [33], based on the seminal work of Booß-Bavnbek and Furutani on infinite-dimensional Lagrangian planes [7, 8, 18].

Let us state our main results for Hill's operators. They extend the previous works [16, 20] and shed a new light on the results by Bräunlich, Graf, and Ortelli in [9]. Some of our results can already be found in the last article. However, the proofs in [9] use the notion of *frames* of solutions. In the present article, we provide proofs which do not rely on this notion, so that we can generalize them to the Schrödinger case, where one cannot construct such frames of solutions.

Let $n \in \mathbb{N} \setminus \{0\}$ be fixed, and let

$$V_t(x) := V(t, x) \colon \mathbb{T}^1 \times \mathbb{R} \to \mathcal{S}_n, \tag{1}$$

be a periodic family of matrix-valued bounded potentials (which are not necessarily periodic in x). Here, $\mathbb{T}^1 \approx [0, 1]$ is the one-dimensional torus, and $\mathcal{S}_n$ denotes the set of $n \times n$ hermitian matrices. We assume that $t \mapsto V_t$ is continuous from $\mathbb{T}^1$ to $L^\infty(\mathbb{R}, \mathcal{S}_n)$. We consider the family of (bulk) Hill's operators

$$h_t := -\partial_{xx}^2 + V_t \quad \text{acting on } L^2(\mathbb{R}, \mathbb{C}^n).$$

For $E \in \mathbb{R}$, we say that E is in the *gap* of the family (h_t) if $E \notin \sigma(h_t)$ for all $t \in \mathbb{T}^1$. We also consider the family of (edge) Hill's operators

$$h^\sharp_{D,t} := -\partial^2_{xx} + V_t \quad \text{acting on } L^2(\mathbb{R}^+, \mathbb{C}^n),$$

with Dirichlet boundary conditions at $x = 0$. While E is not in the spectrum of the bulk operator $\sigma(h_t)$, it may belong to the spectrum of the edge operator $h^\sharp_{D,t}$. In this case, the corresponding eigenstate is called an *edge mode*.

As t runs through $\mathbb{T}^1 \approx [0, 1]$, a spectral flow may appear for the family $h^\sharp_{D,t}$. We denote by $\mathrm{Sf}(h^\sharp_{D,t}, E, \mathbb{T}^1)$ the net number of eigenvalues of $h^\sharp_{D,t}$ going *downwards* in the gap where E lies. We define the index of $(h_t)_{t\in\mathbb{T}^1}$ as this spectral flow:

$$\mathcal{I}(h_t, E) := \mathrm{Sf}(h^\sharp_{D,t}, E, \mathbb{T}^1).$$

Our main theorem is the following (see Theorem 32 for the proof in the Hill's case, and Theorem 44 for the one in the Schrödinger case).

Theorem 1 (Junctions between two channels). *Let $t \mapsto V_{R,t}$ and $t \mapsto V_{L,t}$ be two continuous periodic families of bounded potentials on $\mathbb{R}$. Let $E \in \mathbb{R}$ be in the gap of both corresponding (bulk) Hill's operators $(h_{L,t})$ and $(h_{R,t})$. Let $\chi\colon \mathbb{R} \to [0, 1]$ be any switch function, satisfying $\chi(x) = 1$ for $x < -X$ and $\chi(x) = 0$ for $x > X$ for some $X > 0$, and let*

$$h^\chi_t := -\partial^2_{xx} + V_{L,t}(x)\chi(x) + V_{R,t}(x)(1 - \chi(x)).$$

Then

$$\boxed{\mathrm{Sf}(h^\chi_t, E, \mathbb{T}^1) = \mathcal{I}(h_{R,t}, E) - \mathcal{I}(h_{L,t}, E).}$$

The operator h^χ_t is a domain wall operator. On the far left, we see the potential $V_{L,t}$, while, on the far right, we see $V_{R,t}$, so this operator models a junction between a left potential and a right one. This theorem states that edge modes must appear at the junction if the left and right indices differ.

Plan of the paper. In Section 2, we recall some basic facts on symplectic spaces and self-adjoint extensions of operators. We then prove our results concerning Hill's operators in Section 3, and explain how to adapt the proofs for Schrödinger operators in Section 4.

Notation of the paper. We write $\mathbb{N} := \{1, 2, 3, \dots\}$ and $\mathbb{N}_0 := \{0, 1, 2, 3, \dots\}$. For $z_0 \in \mathbb{C}$ and $r > 0$, we set $B(z, r) := \{z \in \mathbb{C}\colon |z - z_0| < r\}$ the open ball in the complex plane.

For $\Omega \subset \mathbb{R}^d$ an open set, we denote by $L^p(\Omega, \mathbb{C})$ the usual Lebesgue spaces, and by $H^s(\Omega, \mathbb{C})$ the Sobolev ones. The set $H^s_0(\Omega, \mathbb{C})$ is the completion of $C^\infty_0(\Omega, \mathbb{C})$ for the H^s norm.

Let $\mathcal{H}_1$ and $\mathcal{H}_2$ be two Hilbert spaces. For a bounded operator $A\colon \mathcal{H}_1 \to \mathcal{H}_2$, its dual A^* is the map from $\mathcal{H}_2 \to \mathcal{H}_1$ so that

$$\langle x_2, Ax_1\rangle_{\mathcal{H}_2} = \langle A^* x_2, x_1\rangle_{\mathcal{H}_1} \quad \text{for all } x_1 \in \mathcal{H}_1,\ x_2 \in \mathcal{H}_2.$$

The operator A is *unitary* if $A^*A = \mathbb{I}_{\mathcal{H}_1}$ and $AA^* = \mathbb{I}_{\mathcal{H}_2}$.

For E a Banach space, we say that a map $t \mapsto v(t) \in E$ is *continuously differentiable* if $v'(t)$ is well defined in E for all t (that is $\|v'(t)\|_E < \infty$), and if $t \mapsto v'(t)$ is continuous.

2. First facts and notations

2.1. Lagrangian planes in complex Hilbert spaces

Let us first recall some facts on symplectic Banach/Hilbert spaces. In the original work of Maslov [37], popularized by Arnol'd [1], the authors consider *real* Banach spaces E. Following the recent developments, we present the theory for complex Banach spaces.

2.1.1. Basics in symplectic spaces. Let E be a complex Banach space. A symplectic form on E is a non-degenerate continuous sesquilinear form $\omega\colon E \times E \to \mathbb{C}$ such that

$$\omega(x, y) = -\overline{\omega(y, x)} \quad \text{for all } x, y \in E.$$

For ℓ a linear subspace of E, we denote by

$$\ell^\circ := \{x \in E\colon \omega(x, y) = 0 \text{ for all } y \in \ell\}.$$

The space ℓ° is always closed. Such a subspace is called *isotropic* if $\ell \subset \ell^\circ$, *co-isotropic* if $\ell^\circ \subset \ell$, and *Lagrangian* if $\ell = \ell^\circ$. We also say that ℓ is a *Lagrangian plane* in the latter case. The set of all Lagrangian planes of E, sometime called the *Lagrangian–Grassmannian,* is denoted by $\Lambda(E)$.

Example 2 (In $\mathbb{R}^{2n}$). In the *real* Hilbert space $E = \mathbb{R}^n \times \mathbb{R}^n$, the canonical symplectic form is given by (we write $\mathbf{x} = (x, x')$, $\mathbf{y} = (y, y')$, etc., the elements in $\mathbb{R}^n \times \mathbb{R}^n$)

$$\omega(\mathbf{x}, \mathbf{y}) := \langle x, y'\rangle_{\mathbb{R}^n} - \langle x', y\rangle_{\mathbb{R}^n} \quad \text{for all } \mathbf{x}, \mathbf{y} \in \mathbb{R}^n \times \mathbb{R}^n.$$

When $n = 1$, the Lagrangian planes are all the one-dimensional linear subspaces of $\mathbb{R}^2$. Conversely, if $(\mathbb{R}^N, \omega)$ is a symplectic space, then $N = 2n$ is even, and all Lagrangian planes are of dimension n.

Example 3 (In $\mathbb{C}^{2n}$). Similarly, in the *complex* Hilbert space $\mathbb{C}^{2n}$, the canonical symplectic form is given by (we write again $\mathbf{z} = (z, z')$ the elements in $\mathbb{C}^n \times \mathbb{C}^n$)

$$\omega(\mathbf{z}_1, \mathbf{z}_2) := \langle z_1, z_2' \rangle_{\mathbb{C}^n} - \langle z_1', z_2 \rangle_{\mathbb{C}^n} \quad \text{for all } \mathbf{z}_1, \mathbf{z}_2 \in \mathbb{C}^n \times \mathbb{C}^n.$$

When $n = 1$ for instance, the Lagrangian planes are the one-dimensional linear spaces $L = \mathrm{Vect}_{\mathbb{C}}(\mathbf{z})$ with $\mathbf{z} = (z, z')$ satisfying the extra condition $\bar{z}z' \in \mathbb{R}$. Up to a phase, we may always assume $z \in \mathbb{R}$, in which case $z' \in \mathbb{R}$ as well. So, the Lagrangian planes are the one-dimensional subspaces of $\mathbb{C}^2$ of the form $\mathrm{Vect}_{\mathbb{C}}(\mathbf{z})$ with $\mathbf{z} \in \mathbb{R}^2$.

Example 4 (In $\mathbb{C}^N$). Another example is given by the symplectic form

$$\tilde{\omega}(\mathbf{z}_1, \mathbf{z}_2) = \mathrm{i}\langle \mathbf{z}_1, \mathbf{z}_2 \rangle_{\mathbb{C}^N} \quad \text{for all } \mathbf{z}_1, \mathbf{z}_2 \in \mathbb{C}^N.$$

With this symplectic form, a vector $\mathbf{z} \in \mathbb{C}^N$ is never isotropic, since $\tilde{\omega}(\mathbf{z}, \mathbf{z}) = \mathrm{i}\|\mathbf{z}\|^2 \neq 0$ for $z \neq 0$. In particular, $(\mathbb{C}^N, \tilde{\omega})$ does not have Lagrangian subspaces.

We record the following result.

Lemma 5. *If $\ell_1 \subset \ell_1^\circ$ and $\ell_2 \subset \ell_2^\circ$ are two isotropic subspaces with $\ell_1 + \ell_2 = E$, then ℓ_1 and ℓ_2 are Lagrangians, and $\ell_1 \oplus \ell_2 = E$.*

Proof. Since $\ell_1 + \ell_2 = E$, we have $\{0\} = \ell_1^\circ \cap \ell_2^\circ$. In particular, $\ell_1 \cap \ell_2 \subset \ell_1^\circ \cap \ell_2^\circ = \{0\}$ as well, so $\ell_1 \oplus \ell_2 = E$. Let $x \in \ell_1^\circ \subset E$, and write $x = x_1 + x_2$ with $x_1 \in \ell_1$ and $x_2 \in \ell_2$. Since $\ell_1 \subset \ell_1^\circ$, we have $x_2 = x - x_1 \in \ell_1^\circ$ as well, so $x_2 \in \ell_1^\circ \cap \ell_2 \subset \ell_1^\circ \cap \ell_2^\circ = \{0\}$. This proves that $x = x_1 \in \ell_1$, hence $\ell_1^\circ = \ell_1$. The proof for ℓ_2 is similar. ∎

2.1.2. Lagrangian planes of Hilbert spaces and unitaries. In the case where $E = \mathcal{H}_b$ is a Hilbert space, with inner product $\langle \cdot, \cdot \rangle_{\mathcal{H}_b}$, for all $x \in \mathcal{H}_b$, the map

$$T_x \colon y \mapsto \omega(x, y)$$

is linear and bounded. So, by Riesz' representation theorem, there exists $v \in \mathcal{H}_b$ so that $T_x(y) = \langle v, y \rangle_{\mathcal{H}_b}$. We denote by $J^* x := v$ this element. This defines an operator $J^* \colon \mathcal{H}_b \to \mathcal{H}_b$, satisfying

$$\omega(x, y) = \langle J^* x, y \rangle_{\mathcal{H}_b} = \langle x, J y \rangle_{\mathcal{H}_b} \quad \text{for all } x, y \in \mathcal{H}_b.$$

In particular, since ω is bounded, we have

$$\|J y\|_{\mathcal{H}_b}^2 = \langle J y, J y \rangle_{\mathcal{H}_b} = \omega(J y, y) \leq C_\omega \|J y\| \cdot \|y\|,$$

so $\|J y\| \leq C_\omega \|y\|$, and J is a bounded operator. In addition, from the relation

$$\omega(x, y) = -\overline{\omega(y, x)},$$

we get that

$$\langle x, Jy\rangle_{\mathcal{H}_b} = -\langle Jx, y\rangle_{\mathcal{H}_b},$$

that is $J = -J^*$. Finally, since ω is not degenerate, we have $\mathrm{Ker}(J) = \{0\}$.

Example 6. On $\mathbb{C}^{2n}$ with the canonical symplectic form

$$\omega(x, y) = \langle x_1, y_2\rangle_{\mathbb{C}_n} - \langle x_2, y_1\rangle_{\mathbb{C}^n},$$

we have

$$J = \begin{pmatrix} 0_n & \mathbb{I}_n \\ -\mathbb{I}_n & 0_n \end{pmatrix}.$$

Later in the article, we will make the following Assumption A:

Assumption A. $J^2 = -\mathbb{I}_{\mathcal{H}_b}$.

In this case, J is bounded skew self-adjoint with $J^2 = -\mathbb{I}$, and we have

$$\mathcal{H}_b = \mathrm{Ker}(J - \mathrm{i}) \oplus \mathrm{Ker}(J + \mathrm{i}). \tag{2}$$

The hermitian form $-\mathrm{i}\omega$ is positive definite on $\mathrm{Ker}(J - \mathrm{i})$ and negative definite on $\mathrm{Ker}(J + \mathrm{i})$. In addition, for all $x \in \mathrm{Ker}(J - \mathrm{i})$ and all $y \in \mathrm{Ker}(J + \mathrm{i})$, we have

$$\omega(x, x) = \mathrm{i}\|x\|^2_{\mathcal{H}_b}, \quad \omega(y, y) = -\mathrm{i}\|y\|^2_{\mathcal{H}_b}, \quad \omega(x, y) = 0. \tag{3}$$

The following result goes back to Leray in its seminar [34] (see also [7] and [8, Lemmas 2 and 3]). We skip its proof for the sake of brevity.

Lemma 7. *If Assumption A holds, then there is a one-to-one correspondence between the Lagrangian planes ℓ of $\mathcal{H}_b$ and the unitaries U from* $\mathrm{Ker}(J - \mathrm{i})$ *to* $\mathrm{Ker}(J + \mathrm{i})$*, with*

$$\ell = \{x + Ux : x \in \mathrm{Ker}(J - \mathrm{i})\}.$$

Corollary 8. *If* $\dim \mathrm{Ker}(J - \mathrm{i}) \neq \dim \mathrm{Ker}(J + \mathrm{i})$*, then there are no Lagrangian planes. This happens for instance for the symplectic space $(\mathbb{C}^n, \tilde{\omega})$, with $\tilde{\omega}(z, z') = \mathrm{i}\langle z, z'\rangle_{\mathbb{C}^n}$ (see Example 4), for which we have $Jz = \mathrm{i}z$, so* $\mathrm{Ker}(J - \mathrm{i}) = \mathbb{C}^n$ *while* $\mathrm{Ker}(J + \mathrm{i}) = \{0\}$.

The next lemma shows that the crossing of two Lagrangian planes can be read from their respective unitaries (see, e.g., [8, Lemma 2]).

Lemma 9. *Let ℓ_1 and ℓ_2 be two Lagrangian planes of $\Lambda(\mathcal{H}_b)$, with corresponding unitaries U_1 and U_2 from* $\mathrm{Ker}(J - \mathrm{i})$ *to* $\mathrm{Ker}(J + \mathrm{i})$*. Then there is a natural isomorphism*

$$\mathrm{Ker}(U_2^* U_1 - \mathbb{I}_{\mathrm{Ker}(J-\mathrm{i})}) \approx \ell_1 \cap \ell_2.$$

Proof. If $x^- \in \mathrm{Ker}(J-\mathrm{i})$ is such that $U_2^* U_1 x^- = x^-$, then we have $U_1 x^- = U_2 x^-$ in $\mathrm{Ker}(J+\mathrm{i})$, so $x := x^- + U_1 x^- = x^- + U_2 x^-$ is in $\ell_1 \cap \ell_2$. Conversely, if $x \in \ell_1 \cap \ell_2$, then, writing $x = x^- + x^+$, we have $U_1 x^- = U_2 x^-$, so $U_2^* U_1 x^- = x^-$. ∎

2.1.3. Another unitary. In Section 3.1 below, we will consider periodic paths of Lagrangians $\ell_1(t)$ and $\ell_2(t)$, and define the Maslov index of the pair (ℓ_1, ℓ_2). When $\mathcal{H}_b$ is finite dimensional, we will prove that it equals the winding number of the determinant of $U_2^*(t)U_1(t)$. Unfortunately, since U_1 and U_2 are not endomorphism, we cannot split $\det(U_2^* U_1)$ into $\det(U_1)/\det(U_2)$. In this section, we present another one-to-one correspondence between Lagrangian planes and other unitaries (which will be endomorphisms). The results of this section are new to the best of our knowledge.

We now make the stronger assumption that $\mathcal{H}_b$ is of the form $\mathcal{H}_b = \mathcal{H}_1 \times \mathcal{H}_2$, where $\mathcal{H}_1$ and $\mathcal{H}_2$ are two complex Hilbert spaces, and that, relative to this decomposition, J is of the form

Assumption B. $J = \left(\begin{smallmatrix} 0 & V^* \\ -V & 0 \end{smallmatrix}\right)$ for some (fixed) unitary $V\colon \mathcal{H}_1 \to \mathcal{H}_2$.

It implies $J^2 = -\mathbb{I}_{\mathcal{H}_b}$, so Assumption B is stronger assumption than Assumption A. Furthermore, we can identify

$$\mathrm{Ker}(J-\mathrm{i}) = \begin{pmatrix} 1 \\ \mathrm{i}V \end{pmatrix} \mathcal{H}_1, \quad \text{and} \quad \mathrm{Ker}(J+\mathrm{i}) = \begin{pmatrix} 1 \\ -\mathrm{i}V \end{pmatrix} \mathcal{H}_1.$$

Defining the maps $Q_\pm\colon \mathcal{H}_1 \to \mathrm{Ker}(J \pm \mathrm{i})$ by

$$Q_\pm(x) := \frac{1}{\sqrt{2}} \begin{pmatrix} x \\ \mp \mathrm{i} V x \end{pmatrix} \quad \text{for all } x \in \mathcal{H}_1,$$

with dual

$$Q_\pm^* \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} = \frac{1}{\sqrt{2}} (y_1 \pm \mathrm{i} V^* y_2),$$

we can check that $Q_\pm Q_\pm^* = \mathbb{I}_{\mathrm{Ker}(K \pm \mathrm{i})}$ and $Q_\pm^* Q_\pm = \mathbb{I}_{\mathcal{H}_1}$, so $Q_\pm$ are unitaries. In particular, if U is a unitary from $\mathrm{Ker}(J-\mathrm{i})$ to $\mathrm{Ker}(J+\mathrm{i})$, then

$$\mathcal{U} := Q_+^* U Q_-$$

is a unitary from $\mathcal{H}_1$ to itself, hence an endomorphism. In what follows, we use straight letters U for unitaries from $\mathrm{Ker}(J-\mathrm{i}) \to \mathrm{Ker}(J+\mathrm{i})$, and curly letters $\mathcal{U}$ for unitaries of $\mathcal{H}_1$. We therefore proved the following.

Lemma 10. *If Assumption B (hence Assumption A) holds, then there is a one-to-one correspondence between the Lagrangian planes ℓ of $(\mathcal{H}_1 \times \mathcal{H}_2, \omega)$ and the unitaries*

$\mathcal{U}$ of $\mathcal{H}_1$, with

$$\ell = \left\{ \begin{pmatrix} 1 \\ \mathrm{i}V \end{pmatrix} x + \begin{pmatrix} 1 \\ -\mathrm{i}V \end{pmatrix} \mathcal{U} x : x \in \mathcal{H}_1 \right\}.$$

In addition, if ℓ_1 and ℓ_2 are two Lagrangian planes with corresponding unitaries $\mathcal{U}_1$ and $\mathcal{U}_2$, then there is a natural isomorphism

$$\mathrm{Ker}(\mathcal{U}_2^* \mathcal{U}_1 - \mathbb{I}_{\mathcal{H}_1}) \approx \ell_1 \cap \ell_2.$$

2.2. Self-adjoint extensions of Hill's operators

We now review some basic facts on self-adjoint operators (see, e.g., [39, Chapter X.1] for a complete introduction). We first recall some general definitions, and then focus on second order elliptic operators. We show the connection with symplectic spaces using the second Green's identity.

2.2.1. Self-adjoint operators. Let $\mathcal{H}$ be a separable Hilbert space, and let A with dense domain $\mathcal{D}_A$ be any operator on $\mathcal{H}$. In the sequel, we sometime write $(A, \mathcal{D}_A)$. The *adjoint* of $(A, \mathcal{D}_A)$ is denoted by $(A^*, \mathcal{D}_{A^*})$.

For A a symmetric, hence closable, operator on $\mathcal{H}$, we denote by $(A_{\min}, \mathcal{D}_{\min})$ its closure. The adjoint of $(A_{\min}, \mathcal{D}_{\min})$ is denoted by $(A_{\max}, \mathcal{D}_{\max})$. Since A is symmetric, we have $A_{\min} \subset A_{\max}$ ($A_{\max}$ is an extension of $A_{\min}$). The operator $A_{\min}$ is self-adjoint if and only if $\mathcal{D}_{\min} = \mathcal{D}_{\max}$. Otherwise, any self-adjoint extension of A must be of the form $(\widetilde{A}, \widetilde{\mathcal{D}})$ with

$$A_{\min} \subset \widetilde{A} \subset A_{\max},$$

in the sense

$$\mathcal{D}_{\min} \subset \widetilde{\mathcal{D}} \subset \mathcal{D}_{\max}.$$

In particular, once $\mathcal{D}_{\min}$ and $\mathcal{D}_{\max}$ have been identified, the self-adjoint extensions are simply given by domains $\widetilde{\mathcal{D}}$ with $\mathcal{D}_{\min} \subset \widetilde{\mathcal{D}} \subset \mathcal{D}_{\max}$, and the operator $\widetilde{A}$ acts on this domain via

$$\widetilde{A} x := A_{\max} x \quad \text{for all } x \in \widetilde{\mathcal{D}}.$$

We sometime write $(A_{\max}, \widetilde{\mathcal{D}})$ instead of $(\widetilde{A}, \widetilde{\mathcal{D}})$ to insist that only the domain matters.

There are several ways to identify the self-adjoint extensions of A. The original proof by von Neumann [43] uses the Cayley transform. As noticed in [39, Chapter X.1] following [17], the connection with boundary values is not so clear in this approach. Another approach can be found, e.g., in [7, Section 3.1], where the authors give a correspondence between the self-adjoint extensions of A and the Lagrangian planes of the abstract space $\mathcal{D}_{\max}/\mathcal{D}_{\min}$, with the symplectic form

$$\omega([x],[y]) := \langle x, A_{\max} y \rangle_{\mathcal{H}} - \langle A_{\max} x, y \rangle_{\mathcal{H}}, \quad \text{for all } [x],[y] \in \mathcal{D}_{\max}/\mathcal{D}_{\min}.$$

Again, the connection with boundary conditions is not so clear in this setting.

Here, we follow [33] (see also [11]), which is specific to second order elliptic operators. It uses the second Green's identity.

2.2.2. Self-adjoint extensions of Hill's operators on the semi-line. We first present the theory in the case where $A = h$ is a second order ODE (Hill's operator). We postpone the analysis for general second order elliptic operators to Section 4 below.

Let $n \in \mathbb{N}$ and let $V : \mathbb{R} \to \mathcal{S}_n$ be a bounded potential with values in $\mathcal{S}_n$, the set of $n \times n$ hermitian matrices. We consider the Hill's operator

$$h := -\partial_{xx}^2 + V(x) \quad \text{acting on } \mathcal{H} := L^2(\mathbb{R}, \mathbb{C}^n).$$

The bulk operator h with core domain $C_0^\infty(\mathbb{R}, \mathbb{C}^n)$ is symmetric. Since the potential V is bounded, the operator h is essentially self-adjoint, with domain (see [31, Chapter 4])

$$\mathcal{D} := \mathcal{D}_{\min} = \mathcal{D}_{\max} = H^2(\mathbb{R}, \mathbb{C}^n).$$

When restricting this operator to the half line, we obtain the edge operator

$$h^\sharp := -\partial_{xx}^2 + V(x) \quad \text{acting on } \mathcal{H}^\sharp := L^2(\mathbb{R}^+, \mathbb{C}^n).$$

On the core $C_0^\infty(\mathbb{R}^+, \mathbb{C}^n)$, it is symmetric, and its closure has domain

$$\mathcal{D}_{\min}^\sharp := H_0^2(\mathbb{R}^+, \mathbb{C}^n).$$

The adjoint of $(h_{\min}^\sharp, \mathcal{D}_{\min}^\sharp)$ is the operator $(h_{\max}^\sharp, \mathcal{D}_{\max}^\sharp)$ where $h_{\max}^\sharp := -\partial_{xx}^2 + V(x)$ has domain

$$\mathcal{D}_{\max}^\sharp := H^2(\mathbb{R}^+, \mathbb{C}^n).$$

We have $\mathcal{D}_{\min}^\sharp \subsetneq \mathcal{D}_{\max}^\sharp$, so $h^\sharp$ is not essentially self-adjoint. This reflects the fact that some boundary conditions must be chosen at $x = 0$. The particularity of second order elliptic operators comes from the second Green's identity.

Lemma 11 (second Green's identity). *For all* $\phi, \psi \in \mathcal{D}_{\max}^\sharp$,

$$\langle \phi, h_{\max}^\sharp \psi \rangle_{\mathcal{H}^\sharp} - \langle h_{\max}^\sharp \phi, \psi \rangle_{\mathcal{H}^\sharp} = \langle \phi(0), \psi'(0) \rangle_{\mathbb{C}^n} - \langle \phi'(0), \psi(0) \rangle_{\mathbb{C}^n}.$$

This suggests to introduce the boundary space

$$\mathcal{H}_b := \mathbb{C}^n \times \mathbb{C}^n$$

with its canonical symplectic form ω defined in Example 3. We also introduce the map $\mathrm{Tr} \colon \mathcal{D}_{\max}^\sharp \to \mathcal{H}_b$ defined by

$$\mathrm{Tr}(\phi) := (\phi(0), \phi'(0)) \in \mathcal{H}_b \quad \text{for all } \phi \in \mathcal{D}_{\max}^\sharp. \tag{4}$$

With these notations, the second Green's identity reads

$$\langle \phi, h^\sharp_{\max} \psi \rangle_{\mathcal{H}^\sharp} - \langle h^\sharp_{\max} \phi, \psi \rangle_{\mathcal{H}^\sharp} = \omega(\mathrm{Tr}(\phi), \mathrm{Tr}(\psi)) \quad \text{for all } \phi, \psi \in \mathcal{D}^\sharp_{\max}.$$

We denote by $\| \cdot \|_\sharp$ the graph norm of $h^\sharp$, that is

$$\|\phi\|^2_\sharp := \|\phi\|^2_{\mathcal{H}^\sharp} + \|h^\sharp_{\max}\phi\|^2_{\mathcal{H}^\sharp} \quad \text{for all } \phi \in \mathcal{D}^\sharp_{\max}.$$

In the one-dimensional Hill setting, the graph norm is equivalent to the H^2-norm. Recall that a closed extension of $h^\sharp$ has a domain which is closed for this norm.

Lemma 12. *The map* Tr: $(\mathcal{D}^\sharp_{\max}, \| \cdot \|_\sharp) \to \mathcal{H}_b$ *is well defined, continuous and onto.*

Proof. Since V is bounded, we have that the graph norm $\| \cdot \|_\sharp$ is equivalent to the usual $H^2(\mathbb{R}^+, \mathbb{C}^n)$-norm on $\mathcal{D}^\sharp_{\max} = H^2(\mathbb{R}^+, \mathbb{C}^n)$. Rellich embedding shows that

$$H^2(\mathbb{R}^+, \mathbb{C}^n) \hookrightarrow C^1([0, \infty), \mathbb{C}^n)$$

with continuous embedding. This implies that Tr is a bounded linear operator. Let $C, S \in C^\infty(\mathbb{R}^+, \mathbb{R})$ be two compactly supported smooth functions with $C(0) = S'(0) = 1$ and $C'(0) = S(0) = 0$. Given an element $(u, u') \in \mathcal{H}_b$, we have $(u, u') = \mathrm{Tr}(\psi)$ for $\psi(x) := uC(x) + u'S(x) \in \mathcal{D}^\sharp_{\max}$, so Tr is onto. ∎

The next result shows that the self-adjoint extensions of $h^\sharp$ can be seen as Lagrangian planes of $\mathcal{H}_b$.

Theorem 13. *Let $\mathcal{D}^\sharp$ be a domain satisfying $\mathcal{D}^\sharp_{\min} \subset \mathcal{D}^\sharp \subset \mathcal{D}^\sharp_{\max}$, and let $\ell :=$ $\mathrm{Tr}(\mathcal{D}^\sharp)$. The adjoint domain of $(h^\sharp_{\max}, \mathcal{D}^\sharp)$ satisfies $(\mathcal{D}^\sharp)^* = \mathrm{Tr}^{-1}(\ell^\circ)$.*

In particular, $(h^\sharp_{\max}, \mathcal{D}^\sharp)$ is a self-adjoint extension of $h^\sharp$ if and only if

$$\text{there exists } \ell \in \Lambda(\mathcal{H}_b) \text{ so that } \mathcal{D}^\sharp = \mathrm{Tr}^{-1}(\ell).$$

Proof. Since $\mathcal{D}^\sharp_{\min} \subset \mathcal{D}^\sharp \subset \mathcal{D}^\sharp_{\max}$ and $(\mathcal{D}^\sharp_{\max})^* = \mathcal{D}^\sharp_{\min}$, we have $\mathcal{D}^\sharp_{\min} \subset (\mathcal{D}^\sharp)^* \subset \mathcal{D}^\sharp_{\max}$ as well. Let $\psi_0 \in (\mathcal{D}^\sharp)^* \subset \mathcal{D}^\sharp_{\max}$. By definition of the adjoint, and the second Green's identity, we have

$$0 = \langle \psi_0, h^\sharp_{\max}\phi \rangle_{\mathcal{H}^\sharp} - \langle h^\sharp_{\max}\psi_0, \phi \rangle_{\mathcal{H}^\sharp} = \omega(\mathrm{Tr}(\psi_0), \mathrm{Tr}(\phi)) \quad \text{for all } \phi \in \mathcal{D}^\sharp.$$

We deduce that $\mathrm{Tr}(\psi_0) \in \ell^\circ$. So, $\mathrm{Tr}((\mathcal{D}^\sharp)^*) \subset \ell^\circ$, which implies $(\mathcal{D}^\sharp)^* \subset \mathrm{Tr}^{-1}(\ell^\circ)$.

Conversely, let $\psi_0 \in \mathrm{Tr}^{-1}(\ell^\circ)$. By definition of ℓ° and the second Green's identity, we get

$$0 = \omega(\mathrm{Tr}(\psi_0), \mathrm{Tr}(\phi)) = \langle \psi_0, h^\sharp_{\max}\phi \rangle_{\mathcal{H}^\sharp} - \langle h^\sharp_{\max}\psi_0, \phi \rangle_{\mathcal{H}^\sharp} \quad \text{for all } \phi \in \mathcal{D}^\sharp.$$

In particular, the map $T_{\psi_0} \colon \mathcal{D}^\sharp \to \mathbb{C}$ defined by

$$T_{\psi_0} \colon \phi \mapsto \langle \psi_0, h^\sharp_{\max}\phi \rangle_{\mathcal{H}^\sharp} = \langle h^\sharp_{\max}\psi_0, \phi \rangle_{\mathcal{H}^\sharp}$$

is bounded on $\mathcal{D}^\sharp$ with $\|T_{\psi_0}\phi\|_{\mathcal{H}^\sharp} \le \|h^\sharp_{\max}\psi_0\|_{\mathcal{H}^\sharp}\|\phi\|_{\mathcal{H}^\sharp}$. So, ψ_0 is in the adjoint domain $(\mathcal{D}^\sharp)^*$. This proves as wanted that $\mathrm{Tr}^{-1}(\ell^\circ) \subset (\mathcal{D}^\sharp)^*$, and finally $\mathrm{Tr}^{-1}(\ell^\circ) = (\mathcal{D}^\sharp)^*$.

Since Tr is onto, we have $\mathrm{Tr}(\mathrm{Tr}^{-1}(A))$ for all $A \subset \mathcal{H}_b$. On the other hand, if $\mathcal{D}^\sharp$ defines a self-adjoint extension, then we have

$$\mathcal{D}^\sharp = \mathrm{Tr}^{-1}(\ell^\circ), \quad \text{with } \ell := \mathrm{Tr}(\mathcal{D}^\sharp).$$

We deduce that $\ell = \mathrm{Tr}(\mathcal{D}^\sharp) = \mathrm{Tr}(\mathrm{Tr}^{-1}(\ell^\circ)) = \ell^\circ$, hence ℓ is Lagrangian. Conversely, if ℓ is Lagrangian, we can define the domain $\mathcal{D}^\sharp := \mathrm{Tr}^{-1}(\ell)$. We then have $\mathrm{Tr}(\mathcal{D}^\sharp) = \mathrm{Tr}(\mathrm{Tr}^{-1}(\ell)) = \ell$ by surjectivity of Tr again. In particular, the dual domain satisfies $(\mathcal{D}^\sharp)^* = \mathrm{Tr}^{-1}(\ell^\circ) = \mathrm{Tr}^{-1}(\ell) = \mathcal{D}^\sharp$, so $(H^\sharp_{\max}, \mathcal{D}^\sharp)$ is a self-adjoint extension. This concludes the proof. ∎

In what follows, we denote by $(h^\sharp, \ell^\sharp)$ the self-adjoint extensions of $h^\sharp$ with domain $\mathrm{Tr}^{-1}(\ell^\sharp)$.

Before we go on, let us give some examples of Lagrangian planes and their corresponding unitaries $\mathcal{U}$ for some usual self-adjoint extensions. In the Hill's case, we have $\mathcal{H}_b = \mathcal{H}_1 \times \mathcal{H}_2$ with $\mathcal{H}_1 = \mathcal{H}_2 = \mathbb{C}^n$, with the canonical symplectic form. In particular, the unitary V in Assumption B is $V = \mathbb{I}_n$, and the unitaries $\mathcal{U}\colon \mathbb{C}^n \to \mathbb{C}^n$ can be seen as elements of $\mathrm{U}(n)$.

Example 14 (Dirichlet and Neumann boundary conditions). The Dirichlet extension of $h^\sharp$ corresponds to the Lagrangian plane $\ell_D := \{0\} \times \mathbb{C}^n$, and the Neumann one corresponds to $\ell_N := \mathbb{C}^n \times \{0\}$. To identify the corresponding unitary, we note that $(0, u') \in \ell_D$ can be written as

$$\begin{pmatrix} 0 \\ u' \end{pmatrix} = \begin{pmatrix} 1 \\ \mathrm{i} \end{pmatrix}\Big(-\frac{\mathrm{i}}{2}u'\Big) + \begin{pmatrix} 1 \\ -\mathrm{i} \end{pmatrix}\Big(\frac{\mathrm{i}}{2}u'\Big).$$

Comparing with Lemma 10, this gives the unitary $\mathcal{U}_D := -\mathbb{I}_n \in \mathrm{U}(n)$. The proof for Neumann boundary conditions is similar, and we find $\mathcal{U}_N := \mathbb{I}_n \in \mathrm{U}(n)$.

Example 15 (Robin boundary conditions). Consider Θ and Π two hermitian $n \times n$ matrices so that

$$\Theta^* = \Theta, \quad \Pi^* = \Pi, \quad \Theta\Pi = \Pi\Theta, \quad \Theta^2 + \Pi^2 \text{ is invertible.}$$

Let $\ell_{\Theta,\Pi}$ be the subspace

$$\ell_{\Theta,\Pi} := \{(\Theta x, \Pi x) \colon x \in \mathbb{C}^n\} \subset \mathcal{H}_b.$$

We claim that $\ell_{\Theta,\Pi}$ is Lagrangian. Indeed, first we have

$$\begin{aligned}\omega((\Theta x, \Pi x), (\Theta y, \Pi y)) &= \langle \Theta x, \Pi y\rangle_{\mathbb{C}^n} - \langle \Pi x, \Theta y\rangle_{\mathbb{C}^n} \\ &= \langle x, (\Theta\Pi - \Pi\Theta)y\rangle = 0,\end{aligned}$$

so $\ell_{\Theta,\Pi} \subset \ell_{\Theta,\Pi}^{\circ}$. On the other hand, let $(z, z') \in \ell_{\Theta,\Pi}^{\circ}$. We have

$$\langle z, \Pi x\rangle_{\mathbb{C}^n} = \langle z', \Theta x\rangle_{\mathbb{C}^n} \quad \text{for all } x \in \mathbb{C}^n,$$

so

$$\langle \Pi z - \Theta z', x\rangle_{\mathbb{C}^n} = 0 \qquad \text{for all } x \in \mathbb{C}^n.$$

We deduce that $\Pi z = \Theta z'$. In particular, setting $z_0 = (\Theta^2 + \Pi^2)^{-1}(\Theta z + \Pi z')$, we have $z = \Theta z_0$ and $z' = \Pi z_0$, so $(z, z') = (\Theta z_0, \Pi z_0) \in \ell_{\Theta,\Pi}$. This proves that $\ell_{\Theta,\Pi}$ is Lagrangian. This also proves that

$$\ell_{\Theta,\Pi} = \{(z, z') \in \mathbb{C}^n \times \mathbb{C}^n \colon \Pi z = \Theta z'\}.$$

We say that the corresponding self-adjoint extension has the (Θ, Π)-*Robin boundary condition,* namely $\psi \in H^2(\mathbb{R}^+, \mathbb{C}^n)$, if

$$\Pi \psi(0) = \Theta \psi'(0).$$

To identify the corresponding unitary, we remark that

$$\begin{pmatrix} \Theta x \\ \Pi x \end{pmatrix} = \begin{pmatrix} 1 \\ \mathrm{i} \end{pmatrix} \frac{1}{2}(\Theta - \mathrm{i}\Pi)x + \begin{pmatrix} 1 \\ -\mathrm{i} \end{pmatrix} \frac{1}{2}(\Theta + \mathrm{i}\Pi)x.$$

Comparing with Lemma 10, we recognize the unitary

$$\mathcal{U}_{\Theta,\Pi} := (\Theta + \mathrm{i}\Pi)(\Theta - \mathrm{i}\Pi)^{-1} \in \mathrm{U}(n).$$

Note that $A := (\Theta - \mathrm{i}\Pi)$ is invertible, since $A^*A = \Theta^2 + \Pi^2$ is invertible. We recover Dirichlet boundary condition with the pair $(\Theta, \Pi) = (0, \mathbb{I}_n)$ and Neumann boundary condition with $(\Theta, \Pi) = (\mathbb{I}_n, 0)$.

2.3. The Lagrangian planes $\ell^{\pm}(E)$

In the previous section, we linked the boundary conditions at $x = 0$ with the Lagrangian planes of the boundary space $\mathcal{H}_b$. We now focus on the Cauchy solutions of $H\psi = E\psi$. Since we are also interested in the behaviour at $-\infty$, we introduce $\mathcal{H}^{\sharp,\pm} := L^2(\mathbb{R}^{\pm})$ and the maximal domains

$$\mathcal{D}_{\max}^{\sharp,\pm} := H^2(\mathbb{R}^{\pm}, \mathbb{C}^n).$$

The space $\mathcal{D}_{\max}^{\sharp}$ considered previously corresponds to $\mathcal{D}_{\max}^{\sharp,+}$. We also denote by

$$\mathrm{Tr}^{\pm} \colon \mathcal{D}_{\max}^{\sharp,\pm} \to \mathcal{H}_b$$

the corresponding boundary trace operator

$$\mathrm{Tr}^{\pm}(\psi) = (\psi(0), \psi'(0)) \quad \text{for all } \psi \in \mathcal{D}_{\max}^{\sharp,\pm}.$$

Note that, due to the orientation of the line $\mathbb{R}$, the second Green's identity on the left-side reads

$$\langle \phi, h^{\sharp,-}_{\max} \psi \rangle_{\mathcal{H}^{\sharp,-}} - \langle h^{\sharp,-}_{\max} \phi, \psi \rangle_{\mathcal{H}^{\sharp,-}} = -\omega(\mathrm{Tr}^-(\phi), \mathrm{Tr}^-(\psi)) \quad \text{for all } \phi, \psi \in \mathcal{D}^{\sharp,-}_{\max}. \tag{5}$$

We now set

$$\mathcal{S}^{\pm}(E) := \mathrm{Ker}(h^{\sharp,\pm}_{\max} - E) = \{\psi \in \mathcal{D}^{\sharp,\pm}_{\max} : -\psi'' + V\psi = E\psi\},$$

and

$$\ell^{\pm}(E) := \{\mathrm{Tr}^{\pm}(\psi) : \psi \in \mathcal{S}^{\pm}(E)\} \subset \mathcal{H}_b. \tag{6}$$

The solutions in $\mathcal{S}^{\pm}(E)$ can be seen as the set of Cauchy solutions which are square integrable at $\pm\infty$. Thanks to Cauchy's theory for ODEs, elements $\psi^{\pm}$ of $\mathcal{S}^{\pm}(E)$ can be reconstructed from their boundary values $\mathrm{Tr}^{\pm}(\psi^{\pm}) \in \mathcal{H}_b$.

Lemma 16. *For the bulk operator h, we have that for all $E \in \mathbb{R}$,*

$$\dim \mathrm{Ker}(h - E) = \dim(\ell^+(E) \cap \ell^-(E)).$$

In particular, E is an eigenvalue of h if and only if $\ell^+(E) \cap \ell^-(E) \neq \{0\}$.

Proof. We will provide a general proof later (see the proof of Lemma 38), which works in the Schrödinger case. Let us give a short proof using Cauchy's theory.

Let $(u, u') \in \ell^+(E) \cap \ell^-(E)$, and let ψ be the Cauchy solution of $-\psi'' + V\psi = E\psi$ with $\psi(0) = u$ and $\psi'(0) = u'$. By uniqueness of the Cauchy solution, the restriction of ψ on $\mathbb{R}^{\pm}$ is in $\mathcal{S}^{\pm}(E)$. In particular, ψ is square integrable in $\pm\infty$, so $\psi \in L^2(\mathbb{R}, \mathbb{C}^n)$. Then, since V is bounded, $\psi'' = (E - V)\psi$ is also in $L^2(\mathbb{R}, \mathbb{C}^n)$, and ψ is in the domain $H^2(\mathbb{R}, \mathbb{C}^n)$. As it satisfies $(h - E)\psi = 0$, it is an eigenvector of h for the eigenvalue E. Conversely, if ψ is such an eigenvector, then $\mathrm{Tr}(\psi) \in \ell^+(E) \cap \ell^-(E)$. ∎

One can therefore detect eigenvalues as the crossings of $\ell^+(E)$ and $\ell^-(E)$. We now prove that, when E is in the resolvent set of the bulk operator, we have instead $\ell^+(E) \oplus \ell^-(E) = \mathcal{H}_b$. Our proof only uses the fact that the bulk operator h is essentially self-adjoint.

Theorem 17. *For all $E \in \mathbb{R} \setminus \sigma(h)$, the sets $\ell^{\pm}(E)$ are Lagrangian planes of $\mathcal{H}_b$, and*

$$\mathcal{H}_b = \ell^+(E) \oplus \ell^-(E).$$

This shows for instance that there are as many Cauchy's solutions which decay to $+\infty$ as solutions which decay to $-\infty$ (here, they both form subspaces of dimension n). This is somehow reminiscent of the Weyl's criterion [46] (see also [35]).

Again, we postpone the proof to the Schrödinger section (see the proof of Theorem 39 below), as it is similar, but somehow looks more complex in the PDE setting.

Remark 18. In the proof given below, we use that $h = -\partial_{xx}^2 + V$ is self-adjoint on the whole line, and deduce that $\ell^+(E)$ and $\ell^-(E)$ are both Lagrangian planes. Note however that $\ell^+(E)$ is independent of V on $\mathbb{R}^-$. So, $\ell^+(E)$ is a Lagrangian plane whenever there exists an extension of V on $\mathbb{R}^-$ for which the corresponding bulk operator has E in its resolvent set.

Remark 19. The spaces $\ell^\pm(E)$ are not always Lagrangian planes. For instance, if $V: \mathbb{R} \to \mathbb{R}$ is 1-periodic, the spectrum of $h := -\partial_{xx}^2 + V$ is composed of bands and gaps. For $E \in \sigma(h)$, the set of solutions of $(h - E)\psi$ is two-dimensional, and spanned by two quasi-periodic functions, hence the solutions never decay at $\pm\infty$. So, for all $E \in \sigma(h)$, we have $\ell^+(E) = \ell^-(E) = \emptyset$.

At this point, we defined two types of Lagrangian planes for a given operator h. First, we defined the planes $\ell^\sharp$ representing the boundary conditions of a self-adjoint extension of the edge Hamiltonian $h^\sharp$. Then, we defined the planes $\ell^+(E)$ as the set of traces of $\mathrm{Ker}(h^\sharp_{\max} - E)$. If $\mathrm{Tr}(\psi) \in \ell^+(E) \cap \ell^\sharp$, then ψ is in the domain of $h^\sharp$, and satisfies $(h^\sharp - E)\psi = 0$. So, ψ is an eigenvector for the eigenvalue E. This proves the following (compare with Lemma 16).

Lemma 20. *Let $E \in \mathbb{R} \setminus \sigma(h)$, and consider a self-adjoint extension $(h^\sharp, \ell^\sharp)$ of the edge operator. Then*

$$\dim \mathrm{Ker}(h^\sharp - E) = \dim(\ell^+(E) \cap \ell^\sharp).$$

This result is of particular importance, since we detect eigenvalues as the crossing of two Lagrangian planes. The first one $\ell^+(E)$ only depends on bulk properties (e.g., on the potential V), while the second one $\ell^\sharp$ only depends on the chosen boundary conditions at the edge (and is usually independent of the choice of V).

If in addition Assumption B holds, then we can introduce $\mathcal{U}^+(E)$ and $\mathcal{U}^\sharp$ the unitaries corresponding to the Lagrangian planes $\ell^+(E)$ and $\ell^\sharp$ respectively, and we have

$$\dim \mathrm{Ker}(h^\sharp - E) = \dim(\ell^+(E) \cap \ell^\sharp) = \dim((\mathcal{U}^\sharp)^* \mathcal{U}^+(E) - 1).$$

Remark 21 (Scattering coefficients). Let us give an interpretation of the unitary $\mathcal{U}^+(E)$. For $E \notin \sigma(h)$ and $E > 0$, waves cannot propagate in the medium at energy E. Considering the half-medium $-\partial_{xx}^2 + \mathbb{1}(x > 0)V(x)$, any incident wave coming from the left of the form $\mathrm{e}^{\mathrm{i}kx}u$ with $k := \sqrt{E}$ and $u \in \mathbb{C}^n$ "must bounce back." According to scattering theory, there is a unitary operator $R(k) \in \mathrm{U}(n)$, called the *reflection* *coefficient*, so that there is a continuous solution $\psi_u(x)$ of

$$\begin{cases} \psi_u(x) = \mathrm{e}^{\mathrm{i}kx}u + \mathrm{e}^{-\mathrm{i}kx}(R(k)u) & \text{for } x < 0, \\ (-\partial^2_{xx} + V(x))\psi_u(x) = 0 & \text{for } x > 0, \end{cases}$$

and $\psi_u(x)$ is square-integrable at $+\infty$ (no transmission). This shows that $\psi_u \mathbb{1}_{\mathbb{R}^+} \in \mathcal{S}^+(E)$. Taking boundary values, we obtain

$$\begin{pmatrix} (\mathbb{I}_n + R(k))u \\ \mathrm{i}k(\mathbb{I}_n - R(k))u \end{pmatrix} \in \ell^+(E) = \left\{ \begin{pmatrix} 1 \\ \mathrm{i} \end{pmatrix} x + \begin{pmatrix} 1 \\ -\mathrm{i} \end{pmatrix} \mathcal{U}^+(E)x : x \in \mathbb{C}^n \right\} \quad \text{for all } u \in \mathbb{C}^n.$$

This leads to the identity

$$k \cdot \frac{1 - R(k)}{1 + R(k)} = \frac{1 - \mathcal{U}^+(E)}{1 + \mathcal{U}^+(E)}, \quad k = \sqrt{E}.$$

In other words, the Cayley transform of $\mathcal{U}^+(E)$ equals the one of the reflection coefficient $R(k)$, up to the multiplicative factor k.

3. Families of Hill's operators

In the previous section, we exhibit the relationships between self-adjoint extensions, Lagrangian planes, and unitaries. We now consider periodic families of these objects, parameterized by $t \in \mathbb{T}^1$, namely $h^\sharp_t$, $\ell^\sharp_t$ and $\mathcal{U}^\sharp_t$. For each such family, we define an index, namely a *spectral flow* across E for the family $h^\sharp_t$, a *Maslov index* for the bifamily $(\ell^+_t(E), \ell^\sharp_t)$ and a *spectral flow* across 1 for the family $(\mathcal{U}^\sharp_t)^* \mathcal{U}^+_t(E)$. All these objects are defined in the following sections, and we prove that they all coincide.

All these indices can be defined for *continuous* families. However, since the proofs are simpler in the continuously differentiable case, we restrict ourselves to this case. As these indices depend only on the homotopy class of the corresponding loops, similar results hold in the continuous case.

3.1. Families of Lagrangians, and Maslov index

We first define the Maslov index of two families of Lagrangian spaces. This index originates from the work of Maslov in [1, 37]. In these works, the index was defined for finite-dimensional real symplectic spaces (namely $\mathbb{R}^{2n}$ in Example 2). A modern approach can be found in [18], where the infinite-dimensional case is studied as well. Here, we present a simple version of the theory, which is enough for our purpose.

Let $(\mathcal{H}_b, \omega)$ be a symplectic Hilbert space (not necessarily finite dimensional). We define a topology on the Lagrangian Grassmannian $\Lambda(\mathcal{H}_b)$ by setting

$$\operatorname{dist}(\ell_1, \ell_2) := \|P_1 - P_2\|_{\mathrm{op}} \quad \text{for all } \ell_1, \ell_2 \in \Lambda(\mathcal{H}_b),$$

where P_1 and P_2 are the orthogonal projectors on ℓ_1 and ℓ_2 respectively. A family $\ell(t)$ in $\Lambda(\mathcal{H}_b)$ is said *continuous, continuously differentiable,* etc., if the corresponding family of projectors $P(t)$ is so in $\mathcal{B}(\mathcal{H}_b)$.

3.1.1. Definition with quadratic crossing forms. Consider two continuously differentiable families $\mathbb{T}^1 \ni t \mapsto \ell_1(t)$ and $\mathbb{T}^1 \ni t \mapsto \ell_2(t)$. Let $t^* \in \mathbb{T}^1$ be such that $\ell_1(t^*) \cap \ell_2(t^*) \neq \{0\}$. We define the sesquilinear form b on $\ell_1(t^*) \cap \ell_2(t^*)$ by

$$b_{\ell_1,\ell_2}(x, y) := \omega(x, P_1'(t^*)y) - \omega(x, P_2'(t^*)y) \quad \text{for all } x, y \in \ell_1(t^*) \cap \ell_2(t^*). \tag{7}$$

Lemma 22. *The sesquilinear form b_{ℓ_1,ℓ_2} is hermitian: $b_{\ell_1,\ell_2}(x, y) = \overline{b_{\ell_1,\ell_2}(y, x)}$.*

Proof. Let $P_t := P_1(t)$. First, since $\operatorname{Ran} P_1(t) = \ell_1(t)$ is isotropic for all t, we have

$$\omega(P_t(x), P_t(y)) = 0 \quad \text{for all } x, y \in \mathcal{H}_b,\ t \in \mathbb{T}^1.$$

Differentiating gives

$$\omega(P_t(x), P_t'(y)) = -\omega(P_t'(x), P_t(y)) = \overline{\omega(P_t(y), P_t'(x))}.$$

Taking $t = t^*$ and $x, y \in \ell_1(t^*) \cap \ell_2(t^*)$, so that $P_{t^*}(x) = x$ and $P_{t^*}(y) = y$ gives

$$\omega(x, P_t'(y)) = \overline{\omega(y, P_t'(x))} \quad \text{for all } x, y \in \ell_1(t^*) \cap \ell_2(t^*).$$

A similar equality holds for $P_t = P_2(t)$, which proves that b_{ℓ_1,ℓ_2} is hermitian. ∎

In particular, all eigenvalues of b_{ℓ_1,ℓ_2} are real-valued. We say that t^* is a *regular crossing* if $\ell_1(t^*) \cap \ell_2(t^*)$ is finite dimensional (say of dimension $k \in \mathbb{N}$), and if all eigenvalues $(\mu_1, \ldots, \mu_k)$ of b are non-null (so the corresponding quadratic form is non-degenerate). For such crossings, we set

$$\deg(t^*) = \sum_{j=1}^{k} \operatorname{sgn}(\mu_j).$$

The pair $(\ell_1(t), \ell_2(t))$ is regular if all crossings are regular. For such pair, the Maslov index is defined by

$$\boxed{\operatorname{Mas}(\ell_1, \ell_2, \mathbb{T}^1) := \sum_{t^* \text{ regular crossing}} \deg(t^*) \in \mathbb{Z}.}$$

It is clear from the definition that $\operatorname{Mas}(\ell_1, \ell_2, \mathbb{T}^1) = -\operatorname{Mas}(\ell_2, \ell_1, \mathbb{T}^1)$. This definition does not require Assumption A (nor Assumption B).

3.1.2. Definition with the unitaries U. In the case where Assumption A holds, we can relate the Maslov index to a spectral flow. Consider two continuously differentiable loops of Lagrangian $\ell_1(t)$ and $\ell_2(t)$ from $t \in \mathbb{T}^1$ to $\Lambda(\mathcal{H}_b)$. Let $U_1(t)$ and $U_2(t)$ be the corresponding unitaries from $\mathrm{Ker}(J - \mathrm{i})$ to $\mathrm{Ker}(J + \mathrm{i})$. Then U_1 and U_2 are continuously differentiable for the operator norm topology. From Lemma 9, we have that for all $t \in \mathbb{T}^1$,

$$\dim \mathrm{Ker}(U_2(t)^* U_1(t) - \mathbb{I}_{\mathrm{Ker}(J-\mathrm{i})}) = \dim(\ell_1(t) \cap \ell_2(t)).$$

In particular, if all crossings are regular, then $\dim(\ell_1 \cap \ell_2) = \mathrm{Ker}(U_2^* U_1 - 1)$ is finite dimensional. Let $t^* \in \mathbb{T}^1$ be such that the kernel is non-empty, of dimension $k \in \mathbb{N}$. By usual perturbation theory for operators [31], there are k continuously differentiable branches of eigenvalues of the unitary $U_2^* U_1$ crossing 1 around t^*. More specifically, we have the following.

Lemma 23. *Let $U(t)$ be a periodic continuously differentiable family of unitaries, and let $t^* \in \mathbb{T}^1$ be such that*

$$\dim \mathrm{Ker}(U(t^*) - 1) =: k \in \mathbb{N}.$$

Then, there is $\varepsilon > 0$, $\eta > 0$ and k continuously differentiable functions $\{\theta_1(t), \dots, \theta_k(t)\}$ from $t \in (t^* - \varepsilon, t^* + \varepsilon)$ to $\mathbb{S}^1 := \{z \in \mathbb{C} \colon |z| = 1\}$, so that

$$\sigma(U(t)) \cap B(1, \eta) = \{\theta_1(t), \dots, \theta_k(t)\} \cap B(1, \eta).$$

The functions θ_j are the branches of eigenvalues of U. We say that t^* is a *regular crossing* if $k := \dim \mathrm{Ker}(U(t^*) - 1) < \infty$, and if $\theta_j'(t^*) \neq 0$ for all $1 \leq j \leq k$. Note that since θ_j has values in $\mathbb{S}^1$, we have $\theta_j'(t^*) \in \mathrm{i}\mathbb{R}$. The degree of t^* is

$$\deg(t^*) := \sum_{j=1}^{k} \mathrm{sgn}(-\mathrm{i}\theta_j'(t^*)).$$

This is the net number of eigenvalues crossing 1 in $\mathbb{S}^1$ in the positive (counter-clockwise) direction. Finally, if all crossings are regular, the *spectral flow* of U across 1 is

$$\boxed{\mathrm{Sf}(U, 1, \mathbb{T}^1) := \sum_{t^* \text{ regular crossing}} \deg(t^*) \in \mathbb{Z}.}$$

Lemma 24. *Let $\ell_1(t)$ and $\ell_2(t)$ be two continuously differentiable families of Lagrangians in $\Lambda(\mathcal{H}_b)$, and let $U_1(t)$ and $U_2(t)$ be the corresponding unitaries. Then, $t^* \in \mathbb{T}^1$ is a regular crossing of (ℓ_1, ℓ_2) if and only if it is a regular crossing of $U_2^* U_1$. If all crossings are regular, then*

$$\mathrm{Mas}(\ell_1, \ell_2, \mathbb{T}_1) = \mathrm{Sf}(U_2^* U_1, 1, \mathbb{T}^1).$$

Proof. For the sake of simplicity, we assume that only ℓ_1 depends on t. The proof is similar in the general case. Let t^* be a regular crossing point, and let

$$k := \dim(\ell_1(t^*) \cap \ell_2) = \dim \operatorname{Ker}(U_2^* U_1(t^*) - 1).$$

Let $\theta_1, \theta_2, \ldots, \theta_k$ be the branches of eigenvalues crossing 1 at $t = t^*$ (see Lemma 23), and let $x_1^-(t), \ldots, x_k^-(t)$ be a corresponding continuously differentiable set of orthonormal eigenfunctions in $\operatorname{Ker}(J - \mathrm{i})$. First, we have, for all $1 \le i, j \le k$, and all $t \in (t^* - \varepsilon, t^* + \varepsilon)$,

$$\langle x_i^-, [U_2^* U_1(t) - \theta_j] x_j^- \rangle_{\mathcal{H}_b} = 0.$$

Differentiating and evaluating at $t = t^*$ shows that

$$\langle x_i^-, \partial_t [U_2^* U_1 - \theta_j] x_j^- \rangle_{\mathcal{H}_b} + \langle [U_2^* U_1(t^*) - 1]^* x_i^-, (\partial_t x_j^-) \rangle_{\mathcal{H}_b} = 0.$$

At $t = t^*$, we have $U_2^* U_1(t^*) x_i^- = x_i^-$, so $U_1^*(t^*) U_2 x_i^- = x_i^-$ as well, and the last term vanishes. We get the Hellmann–Feynman equation

$$\delta_{ij} \theta_j'(t^*) = \langle U_2 x_i^-, (\partial_t U_1) x_j^- \rangle_{\mathcal{H}_b} |_{t=t^*} = \langle U_1 x_i^-, (\partial_t U_1) x_j^- \rangle_{\mathcal{H}_b} |_{t=t^*}.$$

On the other hand, we set

$$x_j(t) := x_j^-(t) + U_1(t) x_j^-(t) \in \ell_1. \tag{8}$$

We have $x_j \in \ell_1$ for all t, so $P_1 x_j = x_j$ for all t. Differentiating gives

$$(\partial_t P_1) x_j + P_1(\partial_t x_j) = (\partial_t x_j).$$

Since $P_1(\partial_t x_j) \in \ell_1$, which is Lagrangian, we have $\omega(x_i, P_1(\partial_t x_j)) = 0$, so

$$\omega(x_i, (\partial_t P_1) x_j) = \omega(x_i, \partial_t x_j). \tag{9}$$

In addition, differentiating (8) shows that

$$\partial_t x_j = [1 + U_1](\partial_t x_j^-) + (\partial_t U_1) x_j^-.$$

Since $x_j^- \in \operatorname{Ker}(J - \mathrm{i})$ for all t, we have $(\partial_t x_j^-) \in \operatorname{Ker}(J - \mathrm{i})$ as well, and the first term is in ℓ_1. On the other hand, $(\partial_t U_1) x_j^-$ is in $\operatorname{Ker}(J + \mathrm{i})$. Combining with (9) and (3), this gives

$$\omega(x_i, (\partial_t P_1) x_j) = \omega(x_i, \partial_t x_j) = \omega(x_i, (\partial_t U_1) x_j^-) = \omega(U_1 x_i^-, (\partial_t U_1) x_j^-).$$

Using that $\omega(x, y) = \langle x, Jy \rangle_{\mathcal{H}_b}$ and that $(\partial_t U_1) x_j^- \in \operatorname{Ker}(J + \mathrm{i})$, we obtain, at $t = t^*$, and recalling the definition of b in (7),

$$\begin{aligned} b(x_i, x_j) &= \omega(x_i, (\partial_t P_1) x_j) = \omega(U_1 x_i^-, (\partial_t U_1) x_j^-) = \langle U_1 x_i^-, J(\partial_t U_1) x_j^- \rangle \\ &= -\mathrm{i} \langle U_1 x_i^-, (\partial_t U_1) x_j^- \rangle_{\mathcal{H}_b} = \delta_{ij} (-\mathrm{i}) \theta_j'(t^*). \end{aligned}$$

The sesquilinear form b is therefore diagonal in the $(x_1, \ldots, x_k)$ basis, with corresponding eigenvalues $(-\mathrm{i}\theta_j')$. That concludes the proof. ∎

3.1.3. Definition with the unitary $\mathcal{U}$. In the case where the stronger Assumption B holds, one has a similar result with the unitaries $\mathcal{U}$ instead of U. We state it without proof, as it is similar to the previous one.

Lemma 25. *If $(\mathcal{H}_b = \mathcal{H}_1 \times \mathcal{H}_2, \omega)$ satisfies Assumption B. Let $\ell_1(t)$ and $\ell_2(t)$ be two continuously differentiable families of Lagrangian planes in $\Lambda(\mathcal{H}_b)$, and let $\mathcal{U}_1(t)$ and $\mathcal{U}_2(t)$ be the corresponding unitaries of $\mathcal{H}_1$. Then $t^* \in \mathbb{T}^1$ is a regular crossing of (ℓ_1, ℓ_2) if and only if it is a regular crossing of $\mathcal{U}_2^*\mathcal{U}_1$. If all crossings are regular, then,*

$$\mathrm{Mas}(\ell_1, \ell_2, \mathbb{T}_1) = \mathrm{Sf}(\mathcal{U}_2^*\mathcal{U}_1, 1, \mathbb{T}^1).$$

The importance of this lemma comes from the fact that, in the finite-dimensional case ($\mathcal{H}_1 \approx \mathbb{C}^n$), the spectral flow of a periodic family $\mathcal{U}(t) \in \mathrm{U}(n)$ across 1 (or any other point in $\mathbb{S}^1$) equals the winding number of $\det \mathcal{U}(t)$:

$$\mathrm{Sf}(\mathcal{U}, z \in \mathbb{S}^1, \mathbb{T}^1) = \mathrm{Winding}(\det(\mathcal{U}), \mathbb{T}^1).$$

In our case with $\mathcal{U} = \mathcal{U}_2^*\mathcal{U}_1$, we have $\det(\mathcal{U}_2^*\mathcal{U}_1) = \det(\mathcal{U}_1)/\det(\mathcal{U}_2)$, hence

$$\mathrm{Winding}(\det(\mathcal{U}_2^*\mathcal{U}_1), \mathbb{T}^1) = \mathrm{Winding}(\det \mathcal{U}_1, \mathbb{T}^1) - \mathrm{Winding}(\det \mathcal{U}_2, \mathbb{T}^1),$$

that is, the index splits.

Definition 26. For a periodic family of (finite-dimensional) Lagrangians $\ell(t)$ with corresponding unitaries $\mathcal{U}(t)$, we define the index

$$\mathcal{I}(\ell, \mathbb{T}^1) := \mathrm{Winding}(\det(\mathcal{U}(t)), \mathbb{T}^1) \in \mathbb{Z}.$$

We can reformulate Lemma 25 as

$$\mathrm{Mas}(\ell_1, \ell_2, \mathbb{T}^1) = \mathcal{I}(\ell_1, \mathbb{T}^1) - \mathcal{I}(\ell_2, \mathbb{T}^1). \tag{10}$$

3.2. Families of Hill's operators, spectral flow

We now focus on a periodic family of Hill's operators $(h_t)_{t\in\mathbb{T}^1}$. Let $\mathbb{T}^1 \ni t \mapsto V_t$ be a periodic family of potentials satisfying (1), and set

$$h_t := -\partial_{xx}^2 + V_t(x).$$

We assume that $t \mapsto V_t$ is continuously differentiable as a map from $\mathbb{T}^1$ to the Banach space $L^\infty(\mathbb{R}, \mathcal{S}_n)$. Since $\mathbb{T}^1$ is compact, $V(t,x)$ is uniformly bounded. In particular, as in Section 2.2.2, the operator h_t is essentially self-adjoint with fixed domain $\mathcal{D} = H^2(\mathbb{R}^+, \mathbb{C}^n)$ for all $t \in \mathbb{T}^1$.

The *spectrum* of the family $(h_t)_{t \in \mathbb{T}^1}$ is the set

$$\sigma(h_t, \mathbb{T}^1) := \bigcup_{t \in \mathbb{T}^1} \sigma(h_t).$$

It is the compact union of all spectra of (h_t) for $t \in \mathbb{T}^1$. Since $t \mapsto \sigma(h_t)$ is continuous, $\sigma(h_t, \mathbb{T}^1)$ is a closed set in $\mathbb{R}$. The complement of $\sigma(h_t, \mathbb{T}^1)$ is the *resolvent set* of the family $(h_t)_{t \in \mathbb{T}^1}$.

We now consider a corresponding family of edge self-adjoint operators, of the form $(h_t^\sharp, \ell_t^\sharp)$. We say that this family is *continuous, continuously differentiable,* etc., if the corresponding family of Lagrangian planes $\ell_t^\sharp$ is so in $\Lambda(\mathcal{H}_b)$.

Fix $E \in \mathbb{R}$ in the resolvent set of $(h_t)_{t \in \mathbb{T}^1}$. As t varies in $\mathbb{T}^1$, the spectrum of the bulk operator h_t stays away from E. However, for the edge operators $(h_t^\sharp, \ell_t^\sharp)$, some eigenvalues may cross the energy E. If $t^* \in \mathbb{T}^1$ is such that $\dim \mathrm{Ker}(h_{t^*}^\sharp - E) = k \in \mathbb{N}$, then, as in Lemma 23, we can find $\varepsilon > 0$, $\eta > 0$ and k continuously differentiable branches of eigenvalues $\lambda_j(t) \in \mathbb{R}$ so that, for $t \in (t^* - \varepsilon, t^* + \varepsilon)$,

$$\sigma(h_t^\sharp) \cap B(E, \eta) = \{\lambda_1(t), \dots, \lambda_k(t)\} \cap B(E, \eta).$$

At $t = t^*$, we have $\lambda_1(t^*) = \cdots = \lambda_k(t^*) = E$. The crossing t^* is regular if $\lambda_j'(t^*) \neq 0$ for all $1 \le j \le k$. For such a crossing, we set

$$\deg(t^*) = \sum_{j=1}^{k} \mathrm{sgn}(\lambda_j'(t^*)).$$

We say that the energy E is a *regular energy* if all crossings at E are regular. For such an energy, we define the *spectral flow* of $(h_t^\sharp)$ across E as the net number of eigenvalues crossing E downwards (see [2, 38, 45]):

$$\boxed{\mathrm{Sf}(h_t^\sharp, E, \mathbb{T}^1) := - \sum_{t^* \text{regular crossing}} \deg(t^*) \in \mathbb{Z}.}$$

The main result of this section is the following. Recall that the index $\mathcal{I}$ was defined in Definition 26, and that we consider operators on the right half-space.

Theorem 27. *Let $(a, b) \subset \mathbb{R}$ be any interval in $\mathbb{R} \setminus \sigma(h_t, \mathbb{T}_1)$. Then*

- *almost any E in (a, b) is a regular energy for $(h_t^\sharp, \ell_t^\sharp)$;*
- *for any regular energy E in (a, b), we have*

$$\mathrm{Sf}(h_t^\sharp, E, \mathbb{T}^1) = \mathrm{Mas}(\ell_t^+(E), \ell_t^\sharp, \mathbb{T}_1) = \mathcal{I}(\ell_t^+(E), \mathbb{T}^1) - \mathcal{I}(\ell_t^\sharp, \mathbb{T}^1).$$

Proof. The first part comes from Sard's lemma, and can be proved as in [20, Lemma III.18].

Fix E a regular energy, let t^* be a crossing point so that $\dim \mathrm{Ker}(h^\sharp_{t^*} - E) = k \in \mathbb{N}$, and let $\lambda_1, \ldots, \lambda_k$ be the corresponding branches of eigenvalues. The idea of the proof is to follow the two families of branches $(t, \lambda_j(t))$ and (t, E), describing respectively $\ell^\sharp_t$ and $\ell^+_t(E)$.

For the first branch, let $\psi_1(t), \ldots, \psi_k(t)$ be a continuously differentiable family of $\mathcal{H}^\sharp$-orthonormal eigenvectors in

$$\mathcal{D}^\sharp_t := \mathrm{Tr}^{-1}(\ell^\sharp_t)$$

so that

$$h^\sharp_t \psi_j(t) = \lambda_j(t)\psi_j(t), \tag{11}$$

and let

$$u_j := \mathrm{Tr}(\psi_j)$$

so that

$$\ell^+_{t^*}(E) \cap \ell^\sharp_{t^*} = \mathrm{Span}\{u_1(t^*), \ldots, u_k(t^*)\}.$$

For all $t \in (t^* - \varepsilon, t^* + \varepsilon)$, we have (recall that $h^\sharp_t \subset h^\sharp_{t,\max}$)

$$\langle \psi_i(t), (h^\sharp_{t,\max} - \lambda_j(t))\psi_j(t)\rangle_{\mathcal{H}^\sharp} = 0.$$

Differentiating and evaluating at $t = t^*$ gives

$$\begin{aligned} &\langle (\partial_t \psi_i), (h^\sharp_{t^*,\max} - E)\psi_j\rangle_{\mathcal{H}^\sharp}|_{t=t^*} + \langle \psi_i, (h^\sharp_{t^*,\max} - E)(\partial_t \psi_j)\rangle_{\mathcal{H}^\sharp}|_{t=t^*} \\ &\quad + \langle \psi_i, \partial_t (h^\sharp_{t,\max} - \lambda_j)\psi_j\rangle_{\mathcal{H}^\sharp}|_{t=t^*} = 0 \end{aligned}$$

The first term vanishes with (11). For the second term, we put the operator $(h^\sharp_{t^*,\max} - E)$ on the other side using the second Green's identity, and we get

$$\langle \psi_i, (h^\sharp_{t^*,\max} - E)(\partial_t \psi_j)\rangle_{\mathcal{H}^\sharp}|_{t=t^*} = \omega(u_i, \partial_t u_j)|_{t=t^*} = \omega(u_i, (\partial_t P^\sharp_{t^*})u_j)|_{t=t^*}.$$

For the last equality, we introduced $P^\sharp_t$ the projection on $\ell^\sharp_t$, and used an equality similar to (9). This gives our first identity

$$\delta_{ij}\lambda'_j(t^*) = \langle \psi_i, \partial_t (h^\sharp_{t,\max})\psi_j\rangle_{\mathcal{H}^\sharp}|_{t=t^*} + \omega(u_i, \partial_t(P^\sharp_t)u_j)|_{t=t^*}.$$

Remark 28. In the case where the domain $\ell^\sharp_t = \ell^\sharp$ is independent of t, we recover the Hellmann–Feynman identity $\langle \psi_i, \partial_t (h^\sharp_t - \lambda_j)\psi_j\rangle_{\mathcal{H}^\sharp}|_{t=t^*} = 0$.

For the second branch, let $(\phi_1(t), \dots, \phi_k(t))$ be a smooth family of linearly independent functions in $\mathcal{S}_t^+(E)$, and so that, at $t = t^*$, $\phi_j(t^*) = \mathbb{1}_{\mathbb{R}^+}\psi_j(t^*)$. We set

$$v_j = \mathrm{Tr}(\phi_j),$$

so, at $t = t^*$,

$$v_j(t^*) = u_j(t^*).$$

This time, we have, for all $t \in (t^* - \varepsilon, t^* + \varepsilon)$,

$$\langle \phi_i, (h^\sharp_{t,\max} - E)\phi_j \rangle = 0.$$

Differentiating and evaluating at $t = t^*$ gives as before

$$\langle \phi_i, \partial_t (h^\sharp_{t^*,\max})\phi_j \rangle = -\omega(v_i, \partial_t v_j) = -\omega(v_i, (\partial_t P_t^+)v_j) = -\omega(u_i, (\partial_t P_t^+)u_j).$$

Gathering the two identities shows that

$$\delta_{ij}\lambda_j'(t^*) = \omega(u_i, \partial_t(P_t^\sharp)u_j)|_{t=t^*} - \omega(u_i, (\partial_t P_t^+)u_j)|_{t=t^*}.$$

We recognize the sesquilinear form b defined in (7). Actually, we proved that

$$\delta_{ij}\lambda_j'(t^*) = b_{\ell_t^\sharp, \ell_t^+}(u_i, u_j).$$

This form is therefore diagonal in the $(u_1, \dots, u_j)$ basis, and its eigenvalues are the $\lambda_j'(t^*)$. Counting the number of positive/negative $\lambda_j'(t^*)$, and summing over all regular crossings gives as wanted

$$\begin{aligned}\mathrm{Sf}(h_t^\sharp, E, \mathbb{T}^1) &= -\mathrm{Mas}(\ell_t^\sharp, \ell_t^+(E), \mathbb{T}^1) = \mathrm{Mas}(\ell_t^+(E), \ell_t^\sharp, \mathbb{T}^1) \\ &= \mathcal{I}(\ell_t^+(E), \mathbb{T}^1) - \mathcal{I}(\ell_t^\sharp, \mathbb{T}^1).\end{aligned}$$ ■

Remark 29. When considering the operators on the left half line, Green's formula has a minus sign (see equation (5)). The proof is therefore similar up to a sign change, and we get

$$\mathrm{Sf}(h_t^{\sharp,-}, E, \mathbb{T}^1) = -\mathrm{Mas}(\ell_t^-(E), \ell_t^\sharp, \mathbb{T}_1) = \mathcal{I}(\ell_t^\sharp, \mathbb{T}^1) - \mathcal{I}(\ell_t^-(E), \mathbb{T}^1).$$

3.3. Bulk/edge index

Theorem 27 states that the spectral flow of the edge operator $h_t^\sharp$ can be seen as the sum of two contributions: the quantity $\mathcal{I}(\ell_t^+(E), \mathbb{T}^1)$ which only depends on the bulk operator, and the quantity $\mathcal{I}(\ell_t^\sharp, \mathbb{T}^1)$ which only depends on the choice of boundary conditions, so on the nature of the edge. Should we choose the same boundary conditions for all operators $h_t^\sharp$, as it is usually the case, this spectral flow would only depend on the bulk quantity.

So, although the spectral flow is related to edge modes, we emphasize that the index $\mathcal{I}(\ell_t^+(E), \mathbb{T}^1)$ really is a bulk quantity! This motivates the following definition.

Definition 30 (Bulk/edge index). We define the *bulk/edge index* of the family of *bulk* operators $(h_t)_{t\in\mathbb{T}^1}$ at energy $E \notin \sigma(h_t)$ as the spectral flow of its (right) Dirichlet *edge* restriction:

$$\boxed{\mathcal{I}(h_t, E) := \mathrm{Sf}(h_{t,D}^{\sharp,+}, E, \mathbb{T}^1).}$$

Note that we also have $\mathcal{I}(h_t, E) = \mathrm{Mas}(\ell_t^+(E), \ell_D, \mathbb{T}^1) = \mathcal{I}(\ell_t^+(E), \mathbb{T}^1)$ defined in Definition 26. However, our definition of bulk/edge index does no rely on the notion of winding number, as was the case for $\mathcal{I}(\ell_t^+(E), \mathbb{T}^1)$. This definition will therefore works in the infinite-dimensional PDE case, where there is no notion of winding number.

Lemma 31. *When considering the left Dirichlet edge restriction, we have*

$$\mathcal{I}(h_t, E) = -\,\mathrm{Sf}(h_{t,D}^{\sharp,-}, E, \mathbb{T}^1) = \mathcal{I}(\ell_t^-(E), \mathbb{T}^1).$$

Proof. Since $E \notin \sigma(h_t)$ for all $t \in \mathbb{T}^1$, Lemma 16 implies that

$$\ell_t^+(E) \cap \ell_t^-(E) = \{0\} \quad \text{for all } t \in \mathbb{T}^1.$$

So, the Lagrangian planes $\ell_t^+(E)$ and $\ell_t^-(E)$ never cross. In particular,

$$\mathrm{Mas}(\ell_t^+(E), \ell_t^-(E), \mathbb{T}^1) = 0,$$

and therefore

$$\mathcal{I}(\ell_t^+(E), \mathbb{T}^1) = \mathcal{I}(\ell_t^-(E), \mathbb{T}^1).$$

The proof then follows from the fact that $\mathcal{I}(h_t, E) = \mathcal{I}(\ell_t^+(E), \mathbb{T}^1)$ and Remark 29. ■

In Remark 21, we linked the unitary $\mathcal{U}_t^+(E)$ to the reflection coefficient $R_t(k)$ with $k = \sqrt{E}$. Since they have similar Cayley transform (up to a multiplicative positive constant), the winding of $t \mapsto \mathcal{U}_t^+(E)$ equals the one of $t \mapsto R_t(k)$. So, our bulk/edge index is also the winding of the (determinant of the) reflection coefficient $R_t(k)$. The equality

$$\mathrm{Winding}(R_t(k), \mathbb{T}^1) = \mathrm{Sf}(h_{t,D}^{\sharp}, E, \mathbb{T}^1)$$

can be interpreted as a weak (or integrated) form of Levinson's Theorem [41, Theorem XI.59] (see also [22, Theorem 6.11]).

3.4. Applications

Let us give two applications of the previous theory. The first one shows that a spectral flow must appear when modifying Robin boundary conditions. The second one concerns the case of junctions between two Hill's operators.

3.4.1. Robin boundary conditions. In the case $n = 1$, consider a fixed (independent of t) bounded potential $V_t(x) = V(x)$. We consider the self-adjoint Robin operators $h_t^\sharp = -\partial_{xx}^2 + V$ on $L^2(\mathbb{R}^+)$, with the t-dependent domain

$$\mathcal{D}_t := \{\psi \in H^2(\mathbb{R}^+)\colon \sin(\pi t)\psi(0) - \cos(\pi t)\psi'(0) = 0\}.$$

We have $\mathcal{D}_{t+1} = \mathcal{D}_t$, so $H_t^\sharp$ is 1-periodic in t. For $t = 0$, we recover Dirichlet boundary conditions, and for $t = \frac{1}{2}$, we recover Neumann boundary conditions, so Robin boundary conditions interpolates between these two cases. The Lagrangian plane of $\mathcal{H}_b = \mathbb{C} \times \mathbb{C}$ corresponding to the extension $\mathcal{D}_t$ is

$$\ell_t^\sharp = \mathrm{Vect}_{\mathbb{C}} \begin{pmatrix} \cos(\pi t) \\ \sin(\pi t) \end{pmatrix} \subset \mathbb{C} \times \mathbb{C}.$$

It is of the form $\ell_t^\sharp\{(\Theta x, \Pi x)\colon x \in \mathbb{C}\}$ for $\Theta = \cos(\pi t)$ and $\Pi = \sin(\pi t)$. So, by the results of Example 15, the corresponding unitary $\mathcal{U}(t) \in \mathrm{U}(1) \approx \mathbb{S}^1$, is

$$\mathcal{U}(t) = \frac{\cos(\pi t) + \mathrm{i}\sin(\pi t)}{\cos(\pi t) - \mathrm{i}\sin(\pi t)} = \mathrm{e}^{2\mathrm{i}\pi t}.$$

We see that $\mathcal{U}(t)$ winds once positively around $\mathbb{S}^1$ as t runs through $\mathbb{T}^1$, that is,

$$\mathcal{I}(\ell_t^\sharp, \mathbb{T}_1) = 1.$$

Using Theorem 27, and the fact that $\ell_t^+(E)$ is independent of t, we obtain

$$\mathrm{Sf}(h_t^\sharp, E, \mathbb{T}^1) = -1.$$

We deduce that there is a spectral flow of exactly 1 eigenvalue going upwards in all spectral gaps of h. This includes the lower gap $(-\infty, \inf \sigma(h))$.

3.4.2. Junction between two materials. We now consider a junction between a left and a right potentials $V_{L,t}$ and $V_{R,t}$, where $t \mapsto V_{L,t}$ and $t \mapsto V_{R,t}$ are two periodic continuously differentiable families of potentials in $L^\infty(\mathbb{R}, \mathcal{S}_n)$. Take χ a bounded switch function, satisfying, for some $X > 0$,

$$\chi(x) = 1, \text{for all } x \leq -X$$

and

$$\chi(x) = 0 \quad \text{for all } x \geq X.$$

We consider the domain wall Hill's operators

$$h_t^\chi := -\partial_{xx}^2 + V_{L,t}(x)\chi(x) + V_{R,t}(x)(1-\chi(x)).$$

Let $E \in \mathbb{R}$ be in the resolvent set of the bulk operators $h_{R,t}$ and $h_{L,t}$ for all $t \in \mathbb{T}^1$. Again, some eigenvalues of h_t^χ might cross E as t goes from 0 to 1, and we can define a corresponding spectral flow $\mathrm{Sf}(h_t^\chi, E, \mathbb{T}^1)$.

Theorem 32 (Junctions between two channels). *With the previous notation, let*

$$(a,b) \subset \mathbb{R} \setminus \{\sigma(h_{R,t}, \mathbb{T}^1) \cup \sigma(h_{L,t}, \mathbb{T}^1)\}.$$

Then,

- *almost any $E \in (a,b)$ is a regular energy for h_t^χ;*
- *for any such regular energy, we have*

$$\mathrm{Sf}(h_t^\chi, E, \mathbb{T}^1) = \mathcal{I}(h_{R,t}, E) - \mathcal{I}(h_{L,t}, E).$$

In particular, this spectral flow is independent of the switch χ.

Proof. Let us denote by $\ell_{\chi,t}^\pm(x_0, E)$ the Lagrangian planes obtained with the potential

$$V_t^\chi(x) := V_{L,t}(x)\chi(x) + V_{R,t}(x)(1-\chi(x)),$$

and when the real line $\mathbb{R}$ is cut at the location $x_0 \in \mathbb{R}$. By Lemma 16, we have

$$\dim \mathrm{Ker}(h_t^\chi - E) = \dim(\ell_{\chi,t}^+(x_0, E) \cap \ell_{\chi,t}^-(x_0, E)) \quad \text{for all } x_0 \in \mathbb{R}.$$

Adapting the proof of Theorem 27 shows that

$$\begin{aligned}\mathrm{Sf}(h_t^\chi, E, \mathbb{T}^1) &= \mathrm{Mas}(\ell_{\chi,t}^+(x_0, E), \ell_{\chi,t}^-(x_0, E), \mathbb{T}^1) \\ &= \mathcal{I}(\ell_{\chi,t}^+(x_0, E), \mathbb{T}^1) - \mathcal{I}(\ell_{\chi,t}^-(x_0, E), \mathbb{T}^1).\end{aligned}$$

Since V is uniformly (hence locally) bounded, all Cauchy solutions to $-\psi'' + V\psi = E\psi$ are well defined and continuously differentiable on the whole line $\mathbb{R}$. This implies that the maps $x_0 \mapsto \ell_{\chi,t}^\pm(x_0, E)$ are also continuous. In particular, since the index depends only on the homotopy class of the loops, it is independent of $x_0 \in \mathbb{R}$. So

$$\begin{aligned}\mathcal{I}(\ell_{\chi,t}^+(x_0, E), \mathbb{T}^1) &= \mathcal{I}(\ell_{\chi,t}^+(X, E), \mathbb{T}^1) = \mathcal{I}(\ell_{R,t}^+(X, E), \mathbb{T}^1) \\ &= \mathcal{I}(\ell_{R,t}^+(E), \mathbb{T}^1) = \mathcal{I}(h_{R,t}^+, E).\end{aligned}$$

For the middle equality, we used that $\ell_{\chi,t}^+(X, E)$ only involves the half space $\{x \geq X\}$, where we have $V_t^\chi(x) = V_{R,t}(x)$. The proof for the left-hand side is similar, and the result follows from our definition of the bulk/edge index and Lemma 31. ∎

4. The Schrödinger case

In this section, we focus on the PDE Schrödinger case. We chose to put this section separately, since it introduces some technical details, and since the results are slightly different.

4.1. Schrödinger operators on a tube

We consider systems defined on a d-dimensional cylinder of the form

$$\Omega := \mathbb{R} \times \Gamma \subset \mathbb{R}^d,$$

where $\Gamma = (0,1)^{d-1}$ is the $(d-1)$-dimensional unit open square. A point in Ω is denoted by $\mathbf{x} = (x, \mathbf{y})$ with $x \in \mathbb{R}$ and $\mathbf{y} \in \Gamma$.

Let $V : \Omega \to \mathbb{R}$ be a *real-valued* potential, which we assume to be bounded on Ω. We consider bulk Schrödinger operators H of the form

$$H := -\Delta + V, \quad \text{acting on } \mathcal{H} := L^2(\Omega, \mathbb{C}).$$

Again, we do not assume here that V is periodic, but only that V is bounded.

The operator H with core domain $C_0^\infty(\Omega)$ is symmetric, and we have

$$\mathcal{D}_{\min} = H_0^2(\Omega, \mathbb{C}), \quad \text{and} \quad \mathcal{D}_{\max} = H^2(\Omega, \mathbb{C}).$$

This time, the bulk operator is not self-adjoint, and indeed, boundary conditions must be chosen on the boundary of the tube $\partial\Omega = \mathbb{R} \times \partial\Gamma$.

4.1.1. The bulk Schrödinger operators. For the sake of simplicity, we consider periodic boundary conditions. Our results hold for other boundary conditions, such as Dirichlet or Neumann, but the construction of the domains are a bit more technical. So, we rather see Γ as the torus

$$\Gamma := \mathbb{T}^{d-1},$$

so that

$$\Omega := \mathbb{R} \times \mathbb{T}^{d-1}.$$

With this definition, Ω has no boundaries: $\partial\Omega = \emptyset$, and we have $\mathcal{D}_{\min} = \mathcal{D}_{\max} = H^2(\Omega, \mathbb{C})$. The bulk operator H is now self-adjoint (corresponding to the periodic self-adjoint extension).

For $\mathbf{k} \in \mathbb{Z}^{d-1}$, we introduce the $\mathbf{k}$-th Fourier mode $e_{\mathbf{k}}(\mathbf{y}) := \mathrm{e}^{\mathrm{i}2\pi \mathbf{k}\cdot\mathbf{y}}$. The elements in $\mathcal{H}$ can be written in the partial Fourier form

$$f(x, \mathbf{y}) = \sum_{\mathbf{k} \in \mathbb{Z}^{d-1}} f_{\mathbf{k}}(x) e_{\mathbf{k}}(\mathbf{y}), \quad \text{with} \quad \|f\|_{\mathcal{H}}^2 := \sum_{\mathbf{k} \in \mathbb{Z}^{d-1}} \|f_{\mathbf{k}}\|_{L^2(\mathbb{R})}^2 < \infty. \tag{12}$$

A function $f \in \mathcal{H}$ is in the bulk domain $\mathcal{D} := H^2(\Omega, \mathbb{C})$ if $\|(-\Delta) f\|_{\mathcal{H}} < \infty$ as well, where

$$\|(-\Delta) f\|_{\mathcal{H}}^2 = \sum_{\mathbf{k} \in \mathbb{Z}^{d-1}} (\|f_{\mathbf{k}}''\|_{L^2(\mathbb{R})}^2 + (4\pi |\mathbf{k}|^2)^2 \|f_{\mathbf{k}}\|_{L^2(\mathbb{R})}^2) < \infty.$$

4.1.2. Edge Schrödinger operators on a tube. We now define the edge Schrödinger operator

$$H^\sharp := -\Delta + V \quad \text{acting on } L^2(\Omega^+, \mathbb{C}), \text{ where } \Omega^+ := \mathbb{R}^+ \times \mathbb{T}^{d-1}.$$

This operator acts on the right half tube. We sometime write $H^{\sharp,+}$ for $H^\sharp$ and define $H^{\sharp,-}$ for the corresponding operator on the left half tube $\Omega^- := \mathbb{R}^- \times \mathbb{T}^{d-1}$. The operator $H^\sharp$ with core domain $C_0^\infty(\Omega^+)$ is symmetric, and we have

$$\mathcal{D}_{\min}^\sharp = H_0^2(\Omega^+, \mathbb{C}), \quad \text{and} \quad \mathcal{D}_{\max}^\sharp = \{\psi \in L^2(\Omega^+, \mathbb{C}) : (-\Delta + V)\psi \in L^2(\Omega^+, \mathbb{C})\},$$

where the expression $(-\Delta + V)\psi$ must be understood in the distributional sense. Again, we need to specify the boundary conditions at $\partial\Omega^+ = \{0\} \times \mathbb{T}^{d-1}$.

We stress out that the inclusion $H^2(\Omega^+, \mathbb{C}) \subset \mathcal{D}_{\max}^\sharp$ is strict. This makes the PDE setting more tedious to describe. In this section, we focus on domains $\mathcal{D}^\sharp$ which are included in $H^2(\Omega^+, \mathbb{C})$ (this includes the Dirichlet and Neumann extensions). This case is well suited to study junctions, and is much simpler than the general case (with domains in $\mathcal{D}_{\max}^\sharp$). It can be studied as for the Hill's case. We discuss the general case of domains $\mathcal{D}^\sharp \subset \mathcal{D}_{\max}^\sharp$ later in Section 4.5. It is based on a regularized version of Green's identity, and is well suited to study half-systems. However, the general setting is not appropriate to study junctions.

The key ingredient in the case $\mathcal{D}^\sharp \subset H^2(\Omega^+, \mathbb{C})$ is the following.

Lemma 33. *A function is in $H^2(\Omega^+, \mathbb{C})$ if and only if it is the restriction to Ω^+ of an element in the bulk domain $\mathcal{D} = H^2(\Omega, \mathbb{C})$.*

Proof. This follows from the fact that there is an extension operator $H^2(\Omega^+) \to H^2(\Omega)$ which can be constructed with reflection operators, see e.g., [19, Theorem 7.25] or [36, Theorem 8.1]. These reflection operators keep the periodic properties in the last $(d-1)$-directions. ■

4.2. Trace maps, and the boundary space $\mathcal{H}_b$

In order to express the second Green's identity in this setting, we recall some basic facts on the Dirichlet and Neumann trace operators.

4.2.1. Boundary Sobolev-like spaces. Recall that $\Gamma = \mathbb{T}^{d-1}$ is the boundary of Ω^+. For $s \in \mathbb{R}$, we introduce the usual Hilbert spaces $H^s(\Gamma)$, with inner product

$$\langle f, g \rangle_{H^s(\Gamma)} := \sum_{\mathbf{k} \in \mathbb{Z}^{d-1}} \overline{f_{\mathbf{k}}} g_{\mathbf{k}} (1 + (4\pi |\mathbf{k}|)^2)^s,$$

where we introduced the Fourier coefficients

$$f_{\mathbf{k}} = \int_{\mathbb{T}^{d-1}} f(\mathbf{y}) \mathrm{e}^{\mathrm{i}2\pi \mathbf{k}\cdot\mathbf{y}} \mathrm{d}\mathbf{y}.$$

We have $L^2(\Gamma) = H^{s=0}(\gamma)$, and for $s \geq 0$, $H^{-s}(\Gamma)$ is the dual of $H^s(\Gamma)$ for the $L^2(\Gamma)$-inner product. For $s' < s$, we have $H^s(\Gamma) \hookrightarrow H^{s'}(\Gamma)$ with compact embedding, and that $H^s(\Gamma)$ is dense in $H^{s'}(\Gamma)$.

4.2.2. Dirichlet and Neumann trace operators. For $\psi \in C^\infty(\Omega^+)$, we introduce the functions $\gamma^D \psi$ and $\gamma^N \psi$ defined on Γ by

$$(\gamma^D \psi)(\mathbf{y}) := \psi(x = 0, \mathbf{y}), \quad (\gamma^N \psi)(\mathbf{y}) = \partial_x \psi(x = 0, \mathbf{y}) \quad \text{for all } \mathbf{y} \in \Gamma.$$

Our definition differs from the usual one $\gamma^N \psi = -\partial_x \psi(0, \cdot)$, where the minus sign comes from the outward normal direction of Γ from the Ω^+ perspective. Our definition without the minus sign matches the one of the previous section. Finally, we define the trace map

$$\mathrm{Tr}(\psi) = (\gamma^D \psi, \gamma^N \psi). \tag{13}$$

It is classical that Tr can be extended as a bounded operator from $H^2(\Omega^+)$ to $H^{3/2}(\Gamma) \times H^{1/2}(\Gamma)$ (see for instance [36, Theorem 8.3]). This suggests to introduce the boundary space

$$\mathcal{H}_b := H^{3/2}(\Gamma) \times H^{1/2}(\Gamma).$$

The second Green's identity in the PDE case reads as follows.

Lemma 34 (Second Green's formula). *For all $\phi, \psi \in H^2(\Omega^+)$,*

$$\langle \phi, H^\sharp_{\max} \psi \rangle_{\mathcal{H}^\sharp} - \langle H^\sharp_{\max} \phi, \psi \rangle_{\mathcal{H}^\sharp} = \langle \gamma^D \phi, \gamma^N \psi \rangle_{L^2(\Gamma)} - \langle \gamma^N \phi, \gamma^D \psi \rangle_{L^2(\Gamma)}.$$

Introducing the symplectic form ω on $\mathcal{H}_b$, defined by

$$\omega((f, f'), (g, g')) := \langle f, g' \rangle_{L^2(\Gamma)} - \langle f', g \rangle_{L^2(\Gamma)} \qquad \text{for all } (f, f'), (g, g') \in \mathcal{H}_b,$$

the second Green's identity takes the form

$$\langle \phi, H^\sharp_{\max} \psi \rangle_{\mathcal{H}^\sharp} - \langle H^\sharp_{\max} \phi, \psi \rangle_{\mathcal{H}^\sharp} = \omega(\mathrm{Tr}(\phi), \mathrm{Tr}(\psi)) \quad \text{for all } \phi, \psi \in H^2(\Omega^+).$$

Remark 35. The symplectic Hilbert space $(\mathcal{H}_b, \omega)$ *does not* satisfy Assumption A. Introducing the map $A\colon H^{1/2}(\Gamma) \to H^{3/2}(\Gamma)$ so that

$$\langle f, g\rangle_{L^2(\Gamma)} = \langle f, Ag\rangle_{H^{3/2}} = \langle A^* f, g\rangle_{H^{1/2}} \quad \text{for all } f \in H^{3/2}(\Gamma),\ g \in H^{1/2}(\Gamma),$$

we have $J = \left(\begin{smallmatrix} 0 & A^* \\ -A & 0 \end{smallmatrix}\right)$, but the operators A and A^* are compact (hence J as well, and $J^2 \neq -\mathbb{I}_{\mathcal{H}_b}$). In particular, we cannot consider the unitaries U nor $\mathcal{U}$. Such situation, called *weak* symplectic spaces, was studied in [8].

Lemma 36. *The map* $\mathrm{Tr}\colon (H^2(\Omega^+), \|\cdot\|_{H^2}) \to \mathcal{H}_b$ *is well defined, continuous and onto.*

Proof. The fact that Tr is well defined and continuous follows from the continuity of the trace maps. To prove that Tr is onto, one can adapt the proof of [36, Theorem 8.3]. We provide here an alternative short proof.

Let $f \in H^{3/2}(\Gamma)$ and $f' \in H^{1/2}(\Gamma)$ with respective coefficients $(f_{\mathbf{k}})$ and $(f'_{\mathbf{k}})$. Consider also a smooth cut-off function $\chi(x)$ with $\chi(x) = 1$ for $0 \le x < 1/2$, $\chi(x) = 0$ for $x > 2$ and $\int_{\mathbb{R}^+} \chi^2 = 1$. We set $\chi_{\mathbf{0}} = \chi$, and, for $\mathbf{k} \in \mathbb{Z}^{d-1} \setminus \{0\}$,

$$\chi_{\mathbf{k}}(x) := \chi(|\mathbf{k}|x).$$

For all $\mathbf{k}$, the function $\chi_{\mathbf{k}}$ is smooth, compactly supported, with $\chi_{\mathbf{k}}(x) = 1$ for all $x < |\mathbf{k}|/2$. In addition, we have the scalings

$$\int_{\mathbb{R}^+} |\chi_{\mathbf{k}}|^2 = \frac{1}{|\mathbf{k}|}, \quad \int_{\mathbb{R}^+} |\chi'_{\mathbf{k}}|^2 = |\mathbf{k}| \int_{\mathbb{R}^+} |\chi'|^2, \quad \int_{\mathbb{R}^+} |\chi''_{\mathbf{k}}|^2 = |\mathbf{k}|^3 \int_{\mathbb{R}^+} |\chi''|^2.$$

We now consider the function Ψ defined on Ω^+ by

$$\Psi(x, \mathbf{y}) := \sum_{\mathbf{k} \in \mathbb{Z}^{d-1}} (f_{\mathbf{k}} + x f'_{\mathbf{k}}) \chi_{\mathbf{k}}(x) e_{\mathbf{k}}(\mathbf{y}).$$

The function Ψ is smooth with $\mathrm{Tr}(\Psi) = (f, f')$. It remains to check that Ψ is in $H^2(\Omega^+)$. We have for instance

$$\begin{aligned} \|(-\Delta)\Psi\|^2_{L^2(\Omega^+)} &\lesssim \int_{\mathbb{R}^+} \sum_{\mathbf{k} \in \mathbb{Z}^{d-1}} (|f_{\mathbf{k}}|^2 |\mathbf{k}|^4 |\chi_{\mathbf{k}}|^2 + |f_{\mathbf{k}}|^2 |\chi''_{\mathbf{k}}|^2 + |f'_{\mathbf{k}}|^2 |\chi'_{\mathbf{k}}|^2) \\ &\lesssim \sum_{\mathbf{k} \in \mathbb{Z}^{d-1}} |f_{\mathbf{k}}|^2 \cdot |\mathbf{k}|^3 + \sum_{\mathbf{k} \in \mathbb{Z}^{d-1}} |f'_{\mathbf{k}}|^2 |\mathbf{k}| \lesssim \|f\|^2_{H^{3/2}} + \|f'\|^2_{H^{1/2}}. \end{aligned}$$

where we used our previous scalings for $\chi_{\mathbf{k}}$. The L^2–norms of the other derivatives are controlled similarly. ∎

4.2.3. Self-adjointness and Lagrangian spaces. We now provide the counterparts of our previous results in the Schrödinger case. First, we have the following result (compare with Theorem 13).

Theorem 37. *If* $\mathcal{D}^\sharp \subset H^2(\Omega^+)$ *is a domain so that* $(H^\sharp_{\max}, \mathcal{D}^\sharp)$ *is self-adjoint, then* $\ell := \mathrm{Tr}(\mathcal{D}^\sharp)$ *is a Lagrangian plane of* $\mathcal{H}_b$.

Proof. The proof follows the one of Theorem 13. First, the second Green's identity shows that

$$0 = \langle \psi, H^\sharp \phi \rangle - \langle H^\sharp \psi, \phi \rangle = \omega(\mathrm{Tr}(\psi), \mathrm{Tr}(\phi)) \quad \text{for all } \psi, \phi \in \mathcal{D}^\sharp,$$

hence $\ell \subset \ell^\circ$. Conversely, if $\psi_0 \in H^2(\Omega^+)$ is such that $\mathrm{Tr}(\psi_0) \in \ell^\circ$, then for all $\phi \in \mathcal{D}^\sharp$, we have

$$0 = \omega(\mathrm{Tr}(\psi_0), \mathrm{Tr}(\phi)) = \langle \psi_0, H^\sharp \phi \rangle - \langle H^\sharp \psi_0, \phi \rangle.$$

In particular, the map $T_{\psi_0} : \phi \mapsto \langle \psi_0, H^\sharp \phi \rangle = \langle H^\sharp \psi_0, \phi \rangle$ is bounded, with $\| T_{\psi_0} \|_{\mathrm{op}} \leq \| H^\sharp \psi_0 \|_{\mathcal{H}^\sharp}$. So, $\psi_0 \in (\mathcal{D}^\sharp)^* = \mathcal{D}^\sharp$. This proves that $\ell^\circ \subset \mathrm{Tr}(\mathcal{D}^\sharp) \subset \ell$, hence $\ell = \ell^\circ$ is Lagrangian. ∎

Theorem 37 is a much weaker statement than Theorem 13, but is still enough for our purpose (in practice, the self-adjoint extensions are given). There is no longer a one-to-one correspondence between Lagrangian planes and self-adjoint extensions. One problem is that, for $\ell \subset \mathcal{H}_b$, although $\mathrm{Tr}^{-1}(\ell)$ is included in $H^2(\Omega^+)$, its closure for the graph norm $\overline{\mathrm{Tr}^{-1}(\ell)}$ may no longer be included in $H^2(\Omega^+)$. We refer to [6, Example 4.22] for an example of such a situation.

The problem of recovering a function $\psi \in \mathcal{D}^\sharp$ from its boundary value $\mathrm{Tr}(\psi)$ is a well-known problem, often called *boundary value problem,* which has been extensively studied in the literature. The modern tool for this problem is the notion of *boundary triples* [4,5]. In the terminology of the community, we have, in the Hill's case, that $(\mathcal{H}_b := \mathbb{C}^{2n}, \mathrm{Tr}^D, \mathrm{Tr}^N)$ is an ordinary boundary triple, while in the Schrödinger case, $(\mathcal{H}_b = H^{3/2}(\partial\Omega) \times H^{1/2}(\partial\Omega), \mathrm{Tr}^D, \mathrm{Tr}^N)$ is a *quasi*-boundary triple [6]. Below in Section 4.5, we prove a one-to-one correspondence between all self-adjoint extensions and Lagrangian planes of another symplectic Hilbert space of the form $\widetilde{\mathcal{H}_b} = H^{-1/2}(\Gamma) \times H^{1/2}(\Gamma)$. Unfortunately, this construction uses a regularization of the Neumann trace, introduced by Vishik [44] and Grubb [23], and it is not well suited for the study of junctions, as discussed in Section 4.5.

If $\mathcal{D}^\sharp \subset H^2(\Omega^+)$ is a self-adjoint domain, and if $\ell^\sharp = \mathrm{Tr}(\mathcal{D}^\sharp)$ is the corresponding Lagrangian plane, we denote by $(H^\sharp, \ell^\sharp)$ the self-adjoint extensions of $H^\sharp$ corresponding to this Lagrangian plane. Not all $\ell^\sharp \subset \Lambda(\mathcal{H}_b)$ define a self-adjoint domain. As in the finite-dimensional case, we define

$$\mathcal{S}^\pm(E) := \mathrm{Ker}(H^{\sharp,\pm}_{\max} - E) \cap H^2(\Omega^\pm), \quad \text{and} \quad \ell^\pm(E) := \mathrm{Tr}(\mathcal{S}^\pm(E)). \tag{14}$$

The counterpart of Lemma 16 is the following.

Lemma 38. *For the bulk operator H, we have*

$$\dim \operatorname{Ker}(H - E) = \dim(\ell^+(E) \cap \ell^-(E)) \quad \textit{for all } E \in \mathbb{R}.$$

In particular, E is eigenvalue of H if and only if $\ell^+(E) \cap \ell^-(E) \neq \{0\}$.

Proof. If $\psi \in \mathcal{D}$ satisfies $(H - E)\psi = 0$, then, by Lemma 33, its restrictions $\psi^\pm := \mathbb{1}_{\mathbb{R}^\pm}\psi$ are in $H^2(\Omega^\pm)$. In addition, they satisfy $(H^\sharp_{\max} - E)\psi^\pm = 0$, so $\psi^\pm \in \mathcal{S}^\pm(E)$. Taking traces shows that $\operatorname{Tr}^+(\psi^+) = \operatorname{Tr}^-(\psi^-) \in \ell^+(E) \cap \ell^-(E)$.

Conversely, let $\psi^\pm \in \mathcal{S}^\pm(E)$ be such that $\operatorname{Tr}^+(\psi^+) = \operatorname{Tr}^-(\psi^-)$, and consider the function $\psi \in \mathcal{H}$ defined by

$$\psi(x, y) := \begin{cases} \psi^+(x, y) & \text{for } x > 0, \\ \psi^-(x, y) & \text{for } x < 0. \end{cases}$$

It is unclear yet that ψ is regular enough (i.e., belongs to $\mathcal{D} = H^2(\Omega)$). For $f \in \mathcal{D}$, we have

$$\begin{aligned} \langle \psi, (H - E) f \rangle_{\mathcal{H}} &= \langle \psi^+, \mathbb{1}_{\mathbb{R}^+}(H - E) f \rangle_{\mathcal{H}^+} + \langle \psi^-, \mathbb{1}_{\mathbb{R}^-}(H - E) f \rangle_{\mathcal{H}^-} \\ &= \langle \psi^+, (H^{\sharp,+}_{\max} - E) f^+ \rangle_{\mathcal{H}^+} + \langle \psi^-, (H^{\sharp,-}_{\max} - E) f^- \rangle_{\mathcal{H}^-} \\ &= \omega(\operatorname{Tr}^+(\psi^+), \operatorname{Tr}^+(f^+)) - \omega(\operatorname{Tr}^-(\psi^-), \operatorname{Tr}^-(f^-)) = 0. \end{aligned}$$

So, $T_\psi \colon f \mapsto \langle \psi, H f \rangle_{\mathcal{H}} = E\langle \psi, f \rangle_{\mathcal{H}}$ is bounded on $\mathcal{D}$. We first deduce that ψ is in the domain $\mathcal{D}^* = \mathcal{D}$. In addition, we have $(H - E)\psi = 0$. So, ψ is an eigenvector for the eigenvalue E. ∎

Theorem 39. *For all $E \in \mathbb{R} \setminus \sigma(H)$, the sets $\ell^\pm(E)$ are Lagrangian planes of $\mathcal{H}_b$, and*

$$\mathcal{H}_b = \ell^+(E) \oplus \ell^-(E).$$

If $E \in \sigma(H)$, the planes $\ell^\pm(E)$ may not be Lagrangian (see Remark 19).

Proof. We first claim that for any $E \in \mathbb{R}$, $\ell^\pm(E)$ are isotropic spaces. Let $\phi, \psi \in \mathcal{S}^+(E)$. By Green's identity, we have

$$\omega(\operatorname{Tr}(\phi), \operatorname{Tr}(\psi)) = \langle \phi, H^\sharp_{\max}\psi \rangle_{\mathcal{H}^\sharp} - \langle H^\sharp_{\max}\phi, \psi \rangle_{\mathcal{H}^\sharp} = \langle \phi, E\psi \rangle_{\mathcal{H}^\sharp} - \langle E\phi, \psi \rangle_{\mathcal{H}^\sharp} = 0.$$

In the last equality, we used that E is real-valued. This proves that $\ell^+(E) \subset \ell^+(E)^\circ$. Similarly, we have $\ell^-(E) \subset \ell^-(E)^\circ$.

We have (recall that $\mathcal{H} = L^2(\Omega, \mathbb{C}^n)$)

$$\mathcal{H} = \mathcal{H}^+ \oplus \mathcal{H}^-, \quad \text{where } \mathcal{H}^\pm := \{\psi \in \mathcal{H} \colon \psi = 0 \text{ on } \overline{\Omega^\mp}\}.$$

Let $E \in \mathbb{R} \setminus \sigma(H)$, so that the bulk operator $(H - E)$ is invertible with

$$\mathcal{D} = (H - E)^{-1}\mathcal{H}.$$

This gives a decomposition

$$\mathcal{D} = \mathcal{D}^+ \oplus \mathcal{D}^-, \quad \mathcal{D}^\pm := (H - E)^{-1}\mathcal{H}^\pm,$$

and, since Tr is onto,

$$\mathcal{H}_b = \mathrm{Tr}(\mathcal{D}^+) + \mathrm{Tr}(\mathcal{D}^-).$$

The elements $\psi \in \mathcal{D}^+$ are such that $(-\Delta + V - E)\psi = f$, for some $f \in \mathcal{H}$ with support contained in Ω^+. In particular, the restriction of ψ to Ω^-, denoted by ψ^-, is in $H^2(\Omega^-)$ and satisfies $(H^{\sharp,-}_{\max} - E)\psi^- = 0$ on $\mathbb{R}^-$. So, $\psi^- \in \mathcal{S}^-(E)$. Taking boundary traces shows that

$$\mathrm{Tr}(\mathcal{D}^+) \subset \ell^-(E), \quad \text{and, similarly,} \quad \mathrm{Tr}(\mathcal{D}^-) \subset \ell^+(E).$$

In particular, we have $\mathcal{H}_b = \ell^+(E) + \ell^-(E)$. We conclude with Lemma 5. ■

Finally, the counterpart of Lemma 20 is the following. We skip the proof for the sake of brevity.

Lemma 40. *If $E \in \mathbb{R} \setminus \sigma(H)$, then,*

$$\dim \mathrm{Ker}(H^\sharp - E) = \dim(\ell^+(E) \cap \ell^\sharp).$$

In the finite-dimensional Hill's case, for all extensions $(h^{\sharp,+}, \ell^\sharp)$ and $(h^{\sharp,-}, \ell^\sharp)$ with the same Lagrangian plane $\ell^\sharp$, we have

$$\sigma_{\mathrm{ess}}(h) = \sigma_{\mathrm{ess}}(h^{\sharp,+}) \cup \sigma_{\mathrm{ess}}(h^{\sharp,-}).$$

This is because boundary conditions always induce finite-dimensional (hence compact) perturbations of the resolvents. In the Schrödinger case, we only have the inclusion

$$\sigma_{\mathrm{ess}}(H) \subset \sigma_{\mathrm{ess}}(H^{\sharp,+}) \cup \sigma_{\mathrm{ess}}(H^{\sharp,-}),$$

which comes from the fact that Weyl sequences for H must escape to $\pm\infty$. However, the inclusion may be strict: in the infinite-dimensional case, there are self-adjoint extensions of $H^\sharp$ which can create essential spectrum. The corresponding Weyl sequences localize near the cut. We give such an example below in Remark 49.

This makes bulk-boundary correspondence more subtle in the Schrödinger case: different self-adjoint extensions may give different results. For the usual extensions however, we prove that the result are independent of the choice (see the proof of Theorem 44 below).

4.2.4. Families of Schrödinger operators. We consider a family of Schrödinger operators of the form

$$H_t := -\Delta + V_t, \quad \text{acting on } \mathcal{H}.$$

We assume that $t \mapsto V_t$ is continuously differentiable from $\mathbb{T}^1$ to $L^\infty(\Omega, \mathbb{R})$. We also consider a family of (self-adjoint extensions of) edge operators $(H_t^\sharp, \ell_t^\sharp)$.

Let $E \in \mathbb{R} \setminus \sigma(H_t)$. We say that E is a *regular energy* if, for all $t \in \mathbb{T}^1$, the energy E is not in the essential spectrum of $H_t^\sharp$. In particular, this implies

$$\dim \operatorname{Ker}(H_t^\sharp - E) = \dim(\ell_t^+(E) \cap \ell_t^\sharp) < \infty.$$

In addition, we require all corresponding crossings to be regular.

Noticing that the definition of the Maslov index in Section 3.1 does not require Assumption A, we can apply the first part of the proof of Theorem 27 to the Schrödinger case, and we obtain the following.

Theorem 41. *Let $(a, b) \subset \mathbb{R}$ be such that, for all $t \in \mathbb{T}^1$,*

$$(a, b) \cap \sigma(H_t) = \emptyset \quad \text{and} \quad (a, b) \cap \sigma_{\text{ess}}(H_t^\sharp) = \emptyset.$$

Then,

- *almost any $E \in (a, b)$ is a regular energy;*
- *for such a regular energy, we have*

$$\operatorname{Sf}(H_t^\sharp, E, \mathbb{T}^1) = \operatorname{Mas}(\ell_t^+(E), \ell_t^\sharp, \mathbb{T}^1).$$

The proof is similar to the one of Theorem 27, by noticing that all crossings involve finite-dimensional linear spaces. Since the symplectic space $(\mathcal{H}_b, \omega)$ does not satisfy Assumption A, it is unclear whether one can interpret this last index as a spectral flow of unitaries. We postpone this question to Section 4.5 below.

4.3. Junctions for Schrödinger operators

In Section 3.4.2, we proved that the spectral flow for the junctions of two Hill's operators is the difference between a right and a left contributions (the index splits). We prove a similar result for Schrödinger operators.

4.3.1. Bulk/edge index. First we define our bulk/edge index. As in Definition 30, we define it as the spectral flow for the corresponding Dirichlet edge operator.

Definition 42 (Bulk/edge index -bis). We define the *bulk/edge index* of the family of *bulk* operators $(H_t)_{t \in \mathbb{T}^1}$ at energy $E \notin \sigma(H_t)$ as the spectral flow of its (right)

Dirichlet *edge* restriction:

$$\boxed{\mathcal{I}(H_t, E) := \mathrm{Sf}(H_{t,D}^{\sharp,+}, E, \mathbb{T}^1).}$$

Let us prove that this definition indeed makes sense, and in particular that Dirichlet boundary conditions does not create essential spectrum. We set $\ell_D^\sharp := \{0\} \times H^{1/2} \in \Lambda(\mathcal{H}_b)$ the Lagrangian plane corresponding to Dirichlet boundary conditions (that is with domain $H^2(\Omega^+) \cap H_0^1(\Omega^+)$).

Theorem 43. *For all $E \notin \sigma(H_t)$, the spectral flow $\mathrm{Sf}(H_{t,D}^{\sharp,+}, E, \mathbb{T}^1)$ is well defined. In addition, we have*

$$\mathcal{I}(H_t, E) = \mathrm{Sf}(H_{t,D}^{\sharp,+}, E, \mathbb{T}^1) = \mathrm{Mas}(\ell_t^\pm(E), \ell_D^\sharp, \mathbb{T}^1) = -\mathrm{Sf}(H_{t,D}^{\sharp,-}, E, \mathbb{T}^1),$$

Proof. Let $H_{t,D} := -\Delta + V_t$ be the operator acting on $L^2(\Omega) \approx L^2(\Omega^- \cup \Omega^+)$, but with Dirichlet boundary conditions at $\{0\} \times \Gamma$. Since V_t is uniformly bounded, the operators H_t and $H_{t,D}$ are uniformly bounded from below. Consider $\Sigma \in \mathbb{R}$ such that

$$\Sigma < \inf_{t \in \mathbb{T}^1} \inf \sigma(H_t) \quad \text{and} \quad \Sigma < \inf_{t \in \mathbb{T}^1} \inf \sigma(H_{D,t}).$$

We set $R_t := (H_t - \Sigma)^{-1}$ and $R_{t,D} := (H_{t,D} - \Sigma)^{-1}$, which are both bounded operators. It is a standard result (see for instance [41, Theorem XI.79] or [10]) that, for some $m \in \mathbb{N}$, $R_t^m - R_{t,D}^m$ is a compact (even trace-class) operator. In particular, for all $t \in \mathbb{T}^1$, we have

$$\sigma_{\mathrm{ess}}(H_t) = \sigma_{\mathrm{ess}}(H_{t,D}).$$

Let (a, b) denote an essential gap of these operators, and let $E \in (a, b)$ be a regular energy for both operators. We see that a branch of eigenvalues of H_t crosses the energy E downwards if and only if a branch of eigenvalues of $(H_t - \Sigma)^{-m}$ crosses $(E - \Sigma)^{-m}$ upwards. So, we have

$$\mathrm{Sf}(H_t, E, \mathbb{T}^1) = -\mathrm{Sf}(R_t^m, (\Sigma - E)^{-m}, \mathbb{T}^1)$$

and similarly for $H_{t,D}$. Since $E \notin \sigma(H_t)$, we have $\mathrm{Sf}(H_t, E, \mathbb{T}^1) = 0$. Introducing

$$R_t^m(s) := R_t + s(R_{t,D}^m - R_t^m),$$

we see that $s \mapsto R_t^m(s)$ is a continuous family of operators connecting R_t^m and $R_{t,D}^m$. Since for all $s \in [0, 1]$, $R_t^m(s)$ is a compact perturbation of R_t, the essential gap does not close as s varies. We deduce that the spectral flow of $t \mapsto R_t^m(s)$ is independent of s (see for instance [38, Proposition 3] or [21, Lemma 4]). So

$$\mathrm{Sf}(R_t^m, (\Sigma - E)^{-m}, \mathbb{T}^1) = \mathrm{Sf}(R_{t,D}^m, (\Sigma - E)^{-m}, \mathbb{T}^1),$$

which gives

$$0 = \mathrm{Sf}(H_t, E, \mathbb{T}^1) = \mathrm{Sf}(H_{t,D}, E, \mathbb{T}^1).$$

The operator $H_{t,D}$ decouples the left and the right side, so E is an eigenvalue of $H_{t,D}$ if and only if it is an eigenvalue of either $H_{t,D}^{\sharp,+}$ or $H_{t,D}^{\sharp,-}$. Actually, we have

$$\mathrm{Sf}(H_{D,t}, E, \mathbb{T}^1) = \mathrm{Sf}(H_{D,t}^{\sharp,+}, E, \mathbb{T}^1) + \mathrm{Sf}(H_{D,t}^{\sharp,-}, E, \mathbb{T}^1),$$

and the result follows. ∎

4.3.2. Junction case. Let us consider two families of potentials $V_{L,t}$ and $V_{R,t}$, continuously differentiable from $\mathbb{T}^1$ to $L^\infty(\Omega)$. For $\chi\colon \Omega \to [0,1]$ a bounded switch function with $\chi(x, \mathbf{y}) = 1$ for $x < -X$ and $\chi(x, \mathbf{y}) = 0$ for $x > X$, we set

$$H_t^\chi := -\Delta + V_t^\chi(\mathbf{x}), \quad \text{with} \quad V_t^\chi := V_{L,t}\chi + V_{R,t}(1-\chi).$$

As in Section 3.4.2, H_t^χ models a junction between a left and right potential.

We denote by $H_{L,t}$ and $H_{R,t}$ the corresponding left and right Hamiltonians. Let $E \in \mathbb{R}$ be in the resolvent set of both $H_{L,t}$ and $H_{R,t}$ for all $t \in \mathbb{T}^1$, so that the Lagrangian planes $\ell_{L,t}^{\pm}(E)$ and $\ell_{R,t}^{\pm}(E)$ are well defined.

Theorem 44 (Junctions in the Schrödinger case). *Let $(a,b) \subset \mathbb{R}$ be such that, for all $t \in \mathbb{T}^1$,*

$$(a,b) \cap (\sigma(H_{t,R}) \cup \sigma(H_{t,L})) = \emptyset.$$

Then, for all $E \in (a,b)$, we have

$$\mathrm{Sf}(H_t^\chi, E, \mathbb{T}^1) = \mathrm{Mas}(\ell_R^+(E), \ell_L^-(E), \mathbb{T}^1) = \mathcal{I}(H_{R,t}, E) - \mathcal{I}(H_{L,t}, E).$$

This number is independent of χ and of E in the gap.

Proof. We first prove the result for $\chi_0(x) = \mathbb{1}(x<0)$. Reasoning as in the proof of Theorem 43, we obtain

$$\begin{aligned}\mathrm{Sf}(H_t^{\chi_0}, E, \mathbb{T}^1) &= \mathrm{Sf}(H_{t,D}^{\chi_0}, E, \mathbb{T}^1)\\ &= \mathrm{Sf}(H_{t,D}^{\chi_0,\sharp,+}, E, \mathbb{T}^1) + \mathrm{Sf}(H_{t,D}^{\chi_0,\sharp,-}, E, \mathbb{T}^1).\end{aligned}$$

Noticing that $H_{t,D}^{\chi_0,\sharp,+}$ only depends on the right part of the potential, while $H_{t,D}^{\chi_0,\sharp,-}$ depends on the left part, together with our definition of the bulk/edge index, we get

$$\mathrm{Sf}(H_t^{\chi_0}, E, \mathbb{T}^1) = \mathcal{I}(H_{R,t}, E) - \mathcal{I}(H_{L,t}, E).$$

For a general switch function χ, the function $\chi - \chi_0$ is compactly supported. In particular,

$$H_t^\chi - H_t^{\chi_0} = (V_{L,t} - V_{R,t})(\chi - \chi_0),$$

is a compact perturbation of $H_t^{\chi_0}$ for all $t \in \mathbb{T}_1$. Again, by robustness of the spectral flow with respect to compact perturbation, we obtain that

$$\mathrm{Sf}(H_t^{\chi}, E, \mathbb{T}^1) = \mathrm{Sf}(H_t^{\chi_0}, E, \mathbb{T}^1),$$

which is independent of the switch χ. ■

Remark 45 (Neumann boundary condition). We defined the bulk/edge index $\mathcal{I}(H_t, E)$ as the spectral flow of the *Dirichlet* boundary conditions (denoted by $\sharp_D$ here)

$$\mathcal{I}(H_t, E) = \mathrm{Sf}(H_t^{\sharp_D,+}, E, \mathbb{T}^1).$$

One can wonder what happens if one takes another (fixed) boundary condition, say Neumann (denoted by $\sharp_N$). By [41, Theorem XI.80], $R_t^m - R_{N,t}^m$ is also compact for some $m > 0$, where $R_{N,t} := (H_{N,t} - \Sigma)^{-1}$ is defined as $R_{D,t}$, but with Neumann boundary conditions. Following the proof of Theorem 44, we obtain

$$\mathrm{Sf}(H_t^{\chi}, E, \mathbb{T}^1) = \mathrm{Sf}(H_{R,t}^{\sharp_N,+}, E, \mathbb{T}^1) + \mathrm{Sf}(H_{L,t}^{\sharp_N,-}, E, \mathbb{T}^1),$$

Taking $H_{L,t}$ independent of t, dropping the notation R for $H_{R,t}$, and using Theorem 44 shows that

$$\mathrm{Sf}(H_t^{\sharp_N,+}, E, \mathbb{T}^1) = \mathrm{Sf}(H_t^{\sharp_D,+}, E, \mathbb{T}^1).$$

In other words, the bulk/edge index defined with Neumann boundary conditions equals the one with Dirichlet boundary conditions.

This reasoning can be generalized for other boundary conditions, but not all of them (as was the case in the finite-dimensional case), since some extensions might create essential spectrum, as we already mentioned.

4.4. Two-dimensional materials

We now explain how to extend our results for the important case of two-dimensional materials. We write $\mathbf{x} = (x, y) \in \mathbb{R}^2$. Let $V: \mathbb{R}^2 \to \mathbb{R}$ be a $\mathbb{Z}^2$-periodic bounded potential, and let $b: \mathbb{R}^2 \to \mathbb{R}$ be a bounded $\mathbb{Z}^2$-periodic magnetic field. A two-dimensional material with potential V and under the magnetic field b perpendicular to the plane is usually modelled by a Schrödinger operator of the form

$$\widetilde{H} := (-\mathrm{i}\nabla + \mathbf{A}(\mathbf{x}))^2 + V(\mathbf{x}) \quad \text{acting on } L^2(\mathbb{R}^2),$$

where the magnetic vector potential $\mathbf{A} = (A_1, A_2)^T$ satisfies $\partial_x A_2 - \partial_y A_1 = b(\mathbf{x})$. In the case where b only depends on the x-direction $b(\mathbf{x}) = b(x)$ (this is the case for constant magnetic fields for instance), we can choose the gauge

$$\mathbf{A} = (0, A(x))^T, \quad \text{with } A(x) := \int_0^x b(t)\mathrm{d}t.$$

The operator $\widetilde{H}$ then takes the form

$$\widetilde{H} := -\partial^2_{xx} + (-\mathrm{i}\partial_y + A(x))^2 + V(\mathbf{x}).$$

Since the operator $\widetilde{H}$ commutes with $\mathbb{Z}$-translations in the y-direction, one can perform a partial Bloch transform [40] in this direction. One obtains the operators

$$\widetilde{H}_t := -\partial^2_{xx} + (-\mathrm{i}\partial_y + A(x) + 2\pi t)^2 + V(\mathbf{x}),$$

where $k := 2\pi t$ corresponds to the Bloch quasi-momentum in the y-direction. The operators $\widetilde{H}_t$ are essentially self-adjoint on $L^2(\mathbb{R} \times \mathbb{T}^1, \mathbb{C})$, with domain $H^2(\mathbb{R} \times \mathbb{T}^1, \mathbb{C})$. When these operators are cut, we get the operators

$$\widetilde{H}_t^\sharp := -\partial^2_{xx} + (-\mathrm{i}\partial_y + A(x) + 2\pi t)^2 + V(\mathbf{x}), \quad \text{acting on } L^2(\mathbb{R}^+ \times \mathbb{T}^1, \mathbb{C}).$$

These operators are not essentially self-adjoint, and the minimal/maximal domains are respectively given by

$$\widetilde{\mathcal{D}}^\sharp_{\min} = \mathcal{D}^\sharp_{\min} = H^2_0(\Omega^+) \quad \text{and} \quad \widetilde{\mathcal{D}}^\sharp_{\max} = \mathcal{D}^\sharp_{\max} = H^2(\Omega^+),$$

independent of t. Although the kinetic operator now depends on t, it only twists the functions in the direction parallel to the cut. In particular, the second Green's identity in Lemma 34 still holds:

$$\langle \phi, \widetilde{H}_t^\sharp \psi \rangle_{L^2(\Omega^+)} - \langle \widetilde{H}_t^\sharp \phi, \psi \rangle_{L^2(\Omega^+)} = \omega(\mathrm{Tr}\ \phi, \mathrm{Tr}\ \psi) \quad \text{for all } \phi, \psi \in \widetilde{\mathcal{D}}^\sharp_{\max},$$

with the same Tr map and the same ω symplectic form as in the previous section (independent of t).

In particular, all previous results stated for the operators $H_t^\sharp$ also hold for the operators $\widetilde{H}_t^\sharp$. There is a slight abuse of notation concerning the spectral flow: the family $t \mapsto \widetilde{H}_t$ is not periodic but *quasi-periodic*, in the sense that $\widetilde{H}_{t+1}$ is unitary equivalent to $\widetilde{H}_t$:

$$\widetilde{H}_{t+1} = S^* \widetilde{H}_t S,$$

with the unitary S defined by

$$(Sf)(x, y) := \mathrm{e}^{2\mathrm{i}\pi y} f(x, y).$$

A similar relation holds for the Dirichlet edge operator $\widetilde{H}_{t,D}^{\sharp}$, since the Dirichlet domain is invariant by the S operator. The spectra $\sigma(\widetilde{H}_t)$ and $\sigma(\widetilde{H}_{t,D}^{\sharp})$ are still 1-periodic, and we can again define the spectral flow of such quasi-periodic family of operators as the number of eigenvalues going downwards in a gap. This allows to define the bulk/edge index for the operators $\widetilde{H}_t$.

Let us consider a junction between two such materials, of the form

$$\widetilde{H}_t^{\mathrm{junct}} := -\partial_{xx}^2 + (-\mathrm{i}\partial_y + A^{\mathrm{junct}}(x) + 2\pi t)^2 + V^{\mathrm{junct}}(\mathbf{x}),$$

where $A^{\mathrm{junct}}(x)$ and $V^{\mathrm{junct}}(\mathbf{x})$ are so that

$$(A^{\mathrm{junct}}, V^{\mathrm{junct}}) = \begin{cases} (A^L, V^L), & x < -X, \\ (A^R, V^R), & x > X, \end{cases}$$

for some $X > 0$. Defining $\widetilde{H}_t^{L/R} := -\partial_{xx}^2 + (-\mathrm{i}\partial_y + A^{L/R}(x) + 2\pi t)^2 + V^{L/R}(\mathbf{x})$, we can prove as before that, for all $E \notin (\sigma(\widetilde{H}_t^L) \cap \sigma(\widetilde{H}_t^R))$, we have

$$\boxed{\mathrm{Sf}(\widetilde{H}_t^{\mathrm{junct}}, E, \mathbb{T}^1) = \mathcal{I}(\widetilde{H}_t^R, E) - \mathcal{I}(\widetilde{H}_t^L, E).}$$

We do not repeat the proof, as it is similar to the one of Theorem 44.

Example 46 (Landau Hamiltonian). Assume $V = 0$, and $b \in \mathbb{R}^*$ is constant. We are studying the Landau Hamiltonian

$$\widetilde{H} := -\partial_{xx}^2 + (-\mathrm{i}\partial_y + bx)^2 \quad \text{acting on } L^2(\mathbb{R}^2).$$

It is well known that H has a discrete (essential) spectrum $\sigma(H) = |b|(2\mathbb{N}_0 + 1)$. Applying a Bloch transform (instead of the usual Fourier transform) in the y-direction gives the operators

$$\widetilde{H}_t := -\partial_{xx}^2 + (-\mathrm{i}\partial_y + bx + 2\pi t)^2 = -\partial_{xx}^2 + \left(-\mathrm{i}\partial_y + b\left(x + \frac{2\pi t}{b}\right)\right)^2,$$

which are all unitarily equivalent to $\widetilde{H}_{t=0}$, up to the translation $x \mapsto x + \frac{2\pi t}{b}$. We recognize a *charge pumping* phenomenon [42], where the system undergoes a translation in the x–direction of $-\frac{2\pi}{b}$ as t goes from 0 to 1. Let $E \in \mathbb{R} \setminus \sigma(H)$, and let $\mathcal{N}_b(E)$ be the number of Landau bands below E, that is $\mathcal{N}_b(E) = \lceil \frac{1}{2}(\frac{E}{|b|} - 1) \rceil$. Each Landau band has a constant electronic density $\frac{|b|}{2\pi}$, in the sense that there are $\frac{|b|}{2\pi}$ electrons per unit cell in each Landau band. So, as t goes from 0 to 1, the total charge which is pumped below E is $\frac{|b|}{2\pi}\mathcal{N}_b(E) \times (-\frac{2\pi}{b}) = -\,\mathrm{sign}(b)\mathcal{N}_b(E)$. Reasoning as in [21, 26, 27], we deduce that

$$\mathcal{I}(\widetilde{H_t}, E) = -\,\mathrm{sign}(b)\mathcal{N}_b(E) = -\,\mathrm{sign}(b)\left\lceil \frac{1}{2}\left(\frac{E}{|b|} - 1\right)\right\rceil.$$

Let $\widetilde{H}^\sharp$ be the Landau operator on the half space $L^2(\mathbb{R}^+ \times \mathbb{R})$ with Dirichlet (or Neumann) boundary condition at $x = 0$. The previous result shows that, for the family $\widetilde{H}_t^\sharp$, there is a spectral flow of $\mathcal{N}_b(E)$ eigenvalues going upwards (if $b > 0$) or downwards (if $b < 0$) in the gap containing E, as t goes from 0 to 1. In particular, all "bulk" gaps of $\widetilde{H}^\sharp$ are filled with "edge" spectrum, a well-known result [12].

Let $V(x, y)$ be a bounded external potential, $\mathbb{Z}$-periodic in the y variable. For $s > 0$, we denote by

$$\widetilde{H}(s) := -\partial_{xx}^2 + (-\mathrm{i}\partial_y + bx)^2 + sV(x, y).$$

This operator still commutes with $\mathbb{Z}$-translations in the y-variable, so we can apply a partial Bloch transform. For $s_0 > 0$ small enough, E is in the resolvent set of $H(s)$ for all $s \in [0, s_0]$. So, $\mathcal{I}(\widetilde{H_t}(s), E)$ is independent of s (see proof of Theorem 43 above), and $\mathcal{I}(\widetilde{H_t}(s), E) = -\operatorname{sign}(b)\mathcal{N}_b(E)$ as well, for all $s \in [0, s_0]$.

It would be interesting to relate our bulk/edge index $\mathcal{I}(\widetilde{H}_t, E)$ to a bulk index of the operator $\widetilde{H}$ (for instance to a Chern number or Chern marker), in the general case.

4.5. General self-adjoint extensions

In this section, we introduce another symplectic boundary space $(\widetilde{\mathcal{H}_b}, \tilde{\omega})$ and another trace map $\widetilde{\mathrm{Tr}}$, which allows to treat the general case of self-adjoint extensions of $H_{\min}^\sharp$ with domains $\mathcal{D}^\sharp \subset \mathcal{D}_{\max}^\sharp$ (not necessarily included in $H^2(\Omega^+)$).

The main idea of the section is to use a Green's identity involving a regularized Neumann trace. This was first introduced by Vishik [44] and Grubb [23]. We skip most of the proofs of this section, and refer to the monograph [4] for details. Similar ideas have been used in the context of elliptic operators in [13] (see also [14, 15]).

4.5.1. The regularized Green's formula. Recall that

$$\mathcal{D}_{\max}^\sharp = \{\psi \in L^2(\Omega^+) \colon (-\Delta + V)\psi \in L^2(\Omega^+)\}.$$

For any $E \in \mathbb{R}$, we introduce the null space

$$\widetilde{\mathcal{S}_E} := \operatorname{Ker}(\mathcal{D}_{\max}^\sharp - E) = \{\psi \in \mathcal{D}_{\max}^\sharp \colon (-\Delta + V)\psi = E\psi\}.$$

The space $\mathcal{S}_E$ introduced in (14) is $\mathcal{S}_E = \widetilde{\mathcal{S}_E} \cap H^2(\Omega^+)$.

Let $H_D^\sharp$ be the Dirichlet extension of $(-\Delta + V)$ on $L^2(\Omega^+)$, that is with domain $\mathcal{D}_D^\sharp := H^2(\Omega^+) \cap H_0^1(\Omega^+)$, and let $\Sigma \in \mathbb{R} \setminus \sigma(H_D^\sharp)$ be a fixed energy in the resolvent set of $H_D^\sharp$. For $\psi \in \mathcal{D}_{\max}^\sharp$, we set

$$\psi_D := (H_D^\sharp - \Sigma)^{-1}(H_{\max}^\sharp - \Sigma)\psi \in H^2(\Omega^+) \cap H_0^1(\Omega^+),$$

and

$$\psi_\Sigma := \psi - \psi_D = (\mathbb{I} - (H_D^\sharp - \Sigma)^{-1}(H_{\max}^\sharp - \Sigma))\psi.$$

By definition, we have the decomposition $\psi = \psi_D + \psi_\Sigma$. In addition, we have

$$(H_{\max}^\sharp - \Sigma)\psi_\Sigma = 0,$$

hence $\psi_\Sigma \in \widetilde{\mathcal{S}_\Sigma}$. This gives a decomposition

$$\mathcal{D}_{\max}^\sharp = \mathcal{D}_D^\sharp + \widetilde{\mathcal{S}_\Sigma}, \quad \psi = \psi_D + \psi_\Sigma.$$

For $\psi = \psi_D + \psi_\Sigma$ a smooth function, we define the *regularized* trace-map

$$\boxed{\widetilde{\mathrm{Tr}}(\psi) := (\gamma^D \psi, \gamma^N \psi_D).}$$

The term "regularized" comes from the fact that only the ψ_D part appears in the Neumann trace. Since $\gamma^D \psi_D = 0$, the Dirichlet trace is also $\gamma^D \psi = \gamma^D \psi_\Sigma$.

Lemma 47. *The map* $\widetilde{\mathrm{Tr}}$ *can be extended as a bounded map from* $\mathcal{D}_{\max}^\sharp$ *(equipped with the graph norm) to the boundary space*

$$\widetilde{\mathcal{H}_b} := H^{-1/2}(\Gamma) \times H^{1/2}(\Gamma).$$

This extension $\widetilde{\mathrm{Tr}}\colon \mathcal{D}_{\max}^\sharp \to \widetilde{\mathcal{H}_b}$ *is surjective. The following Green's identity holds: for all* $\phi, \psi \in \mathcal{D}_{\max}^\sharp$*, we have*

$$\langle \phi, H_{\max}^\sharp \psi \rangle - \langle H_{\max}^\sharp \phi, \psi \rangle = \langle \gamma^D \phi, \gamma^N \psi_D \rangle_{H^{-1/2}, H^{1/2}} - \langle \gamma^N \phi_D, \gamma^D \psi \rangle_{H^{1/2}, H^{-1/2}}.$$

We refer to [4, Theorem 8.4.1] for the proof. Here, $\langle \cdot, \cdot \rangle_{H^{-1/2}, H^{1/2}}$ denotes the duality product.

We introduce the symplectic form $\tilde{\omega}\colon \widetilde{\mathcal{H}_b} \times \widetilde{\mathcal{H}_b} \to \mathbb{C}$ defined by

$$\begin{aligned} &\tilde{\omega}((f, f'), (g, g')) \\ &\quad := \langle f, g' \rangle_{H^{-1/2}, H^{1/2}} - \langle f', g \rangle_{H^{1/2}, H^{-1/2}} \quad \text{for all } (f, f'), (g, g') \in \widetilde{\mathcal{H}_b}. \end{aligned}$$

One can check that $(\widetilde{\mathcal{H}_b}, \tilde{\omega})$ is a symplectic Hilbert space. With this, the Green's identity takes the form

$$\langle \phi, H_{\max}^\sharp \psi \rangle - \langle H_{\max}^\sharp \phi, \psi \rangle = \tilde{\omega}(\widetilde{\mathrm{Tr}}(\phi), \widetilde{\mathrm{Tr}}(\psi)) \quad \text{for all } \phi, \psi \in \mathcal{D}_{\max}^\sharp.$$

Unlike the previous Tr map in (13), the $\widetilde{\mathrm{Tr}}$ map now depends on the operator $H_{\max}^\sharp$ and on the choice of Σ.

4.5.2. General self-adjoint extensions. Since the trace map $\widetilde{\mathrm{Tr}}$ is continuous and onto, one can repeat the arguments of Theorem 13. We obtain the following.

Theorem 48. *Let $\mathcal{D}^\sharp$ be a domain satisfying $\mathcal{D}^\sharp_{\min} \subset \mathcal{D}^\sharp \subset \mathcal{D}^\sharp_{\max}$ and let $\ell := \widetilde{\mathrm{Tr}}(\mathcal{D}^\sharp)$. Then the adjoint domain is $(\mathcal{D}^\sharp)^* = \widetilde{\mathrm{Tr}}^{-1}(\ell^\circ)$.*

In particular, $(H^\sharp_{\max}, \mathcal{D}^\sharp)$ is a self-adjoint extension if and only if

$$\text{there exists } \ell \in \Lambda(\widetilde{\mathcal{H}_b}) \text{ so that } \mathcal{D}^\sharp = \widetilde{\mathrm{Tr}}^{-1}(\ell).$$

This gives a one-to-one correspondence between all self-adjoint extensions of $(-\Delta + V)$ on the half-tube $L^2(\Omega^+)$, and the Lagrangian planes of $(\widetilde{\mathcal{H}_b}, \tilde{\omega})$.

The symplectic space $(\widetilde{\mathcal{H}_b}, \tilde{\omega})$ satisfies Assumption B (hence Assumption A). Indeed, let $V: H^{1/2}(\Gamma) \to H^{-1/2}(\Gamma)$ be the map such that for all $f \in H^{1/2}(\Gamma)$ and all $g \in H^{-1/2}(\Gamma)$, we have

$$\langle f, g\rangle_{H^{1/2}, H^{-1/2}} = \langle f, V^* g\rangle_{H^{1/2}} = \langle Vf, g\rangle_{H^{-1/2}}. \tag{15}$$

The existence of such map V comes from Riesz' Lemma, and we can check that V is unitary. This time, we have $J = \begin{pmatrix} 0 & V \\ -V^* & 0 \end{pmatrix}$, which satisfies Assumption B.

In particular, the Lagrangian planes of $(\widetilde{\mathcal{H}_b}, \tilde{\omega})$ are in one-to-one correspondence with the unitaries $\widetilde{\mathcal{U}}$ of $H^{-1/2}(\Gamma)$ with

$$\tilde{\ell} = \left\{ \begin{pmatrix} 1 \\ \mathrm{i}V^* \end{pmatrix} f + \begin{pmatrix} 1 \\ -\mathrm{i}V^* \end{pmatrix} \widetilde{\mathcal{U}} f : f \in H^{-1/2}(\Gamma) \right\}.$$

As the Hilbert space $H^{-1/2}(\Gamma)$ is unitary equivalent to $L^2(\Gamma)$ and to $H^{1/2}(\Gamma)$, one has similar one-to-one correspondence replacing $H^{-1/2}(\Gamma)$ by $L^2(\Gamma)$ or $H^{1/2}(\Gamma)$.

4.5.3. The planes $\tilde{\ell}(E)$. Let us now focus on the boundary traces of

$$\widetilde{\mathcal{S}_E} = \mathrm{Ker}(H^\sharp_{\max} - E).$$

For $E \in \mathbb{R}$, we introduce the planes

$$\tilde{\ell}(E) := \widetilde{\mathrm{Tr}}(\widetilde{\mathcal{S}_E}) \subset \widetilde{\mathcal{H}_b}.$$

Remark 49. The plane $\ell_D := \{0\} \times H^{1/2}(\Gamma)$ is Lagrangian, and corresponds to the Dirichlet extension. However, the plane $\ell_\Sigma := H^{-1/2}(\Gamma) \times \{0\}$ is Lagrangian, but does not correspond to the Neumann extension. It rather corresponds to $\tilde{\ell}(E = \Sigma)$. The self-adjoint extension corresponding to the Lagrangian plane ℓ_Σ has Σ as an eigenvalue of infinite multiplicities (hence Σ is in its essential spectrum).

The counterpart of Theorem 39 is the following.

Theorem 50. *For all $E \in \mathbb{R} \setminus \sigma_{\mathrm{ess}}(H^\sharp_D)$, $\tilde{\ell}(E)$ is a Lagrangian plane of $(\widetilde{\mathcal{H}_b}, \tilde{\omega})$.*

Unlike Theorem 39, only the essential spectrum of $H_D^\sharp$ matters. This result is independent of the value of V on the left side Ω^- (see Remark 18).

Proof. First, it is clear that $\tilde{\ell}(E)$ is isotropic (see the proof of Theorem 39).

Case 1: E is in the resolvent set. Let us first prove the result for $E \in \mathbb{R} \setminus \sigma(H_D^\sharp)$. In this case, the proof follows the lines of [4, Proposition 8.4.4].

Let $(f, f') \in \tilde{\ell}(E)$, and let $\psi_E \in \widetilde{\mathcal{S}_E}$ be such that $\widetilde{\mathrm{Tr}}(\psi_E) = (f, f')$. Write $\psi_E = \psi_D + \psi_\Sigma$ with $\psi_D \in \mathcal{D}_D^\sharp$ and $\psi_\Sigma \in \widetilde{\mathcal{S}_\Sigma}$. Applying $(H_{\max}^\sharp - E)$ shows that

$$0 = (H_D^\sharp - E)\psi_D + (\Sigma - E)\psi_\Sigma, \quad \text{hence} \quad \psi_D = (E - \Sigma)(H_D^\sharp - E)^{-1}\psi_\Sigma.$$

So

$$\psi_E = (1 + (E - \Sigma)(H_D^\sharp - E)^{-1})\psi_\Sigma.$$

In particular, we have

$$f = \gamma^D \psi_E = \gamma^D \psi_\Sigma, \quad \text{and} \quad f' = \gamma^N \psi_D = (E - \Sigma)\gamma^N (H_D^\sharp - E)^{-1}\psi_N. \tag{16}$$

Recall that $\widetilde{\mathrm{Tr}}$ is bijective from $\mathcal{D}_{\max}^\sharp$ to $H^{-1/2}(\Gamma) \times H^{1/2}(\Gamma)$, and set

$$G_\Sigma(f) := \widetilde{\mathrm{Tr}}^{-1}(f, 0).$$

By decomposing $G_\Sigma(f)$ as $G_\Sigma(f) = g_D + g_\Sigma$, one must have $\gamma^N(g_D) = 0$ with $g_D \in \mathcal{D}_D^\sharp$. This implies $g_D = 0$ by the unique continuation principle, so $G_\Sigma(f) = g_\Sigma \in \widetilde{\mathcal{S}_\Sigma}$. In other words, G_Σ is the map from $H^{-1/2}(\Gamma)$ to $\widetilde{\mathcal{S}_\Sigma}$ so that $\gamma^D(G_\Sigma f) = f$ (this map is called the *γ-field*).

The first equation of (16) reads $\psi_\Sigma = G_\Sigma f$, and the second shows that

$$f' = M(E)f, \quad \text{with} \quad M(E) := (E - \Sigma)\gamma^N (H_D^\sharp - E)^{-1} G_\Sigma.$$

The map $M(E)\colon H^{-1/2}(\Gamma) \to H^{1/2}(\Gamma)$ is called the *Weyl M-function.*

Conversely, let $f \in H^{-1/2}(\Gamma)$, and set $f' = M(E)f$. By defining

$$\psi_E := (1 + (E - \Sigma)(H_D^\sharp - E)^{-1})G_\Sigma f,$$

we can check that $\psi_E \in \widetilde{\mathcal{S}_E}$ and $\widetilde{\mathrm{Tr}}(\Psi_E) = (f, f')$. So, $(f, f') \in \tilde{\ell}(E)$. This proves that

$$\tilde{\ell}(E) = \{(f, M(E)f) \colon f \in H^{-1/2}(\Gamma)\},$$

that is $\tilde{\ell}(E)$ is the graph of the map $M(E)$.

The map $M(E)$ is a bounded operator from $H^{-1/2}(\Gamma)$ to $H^{1/2}(\Gamma)$. The fact that $\tilde{\ell}(E)$ is isotropic is equivalent to the fact that $M(E)$ is symmetric, in the sense

$$\langle f, M(E)g\rangle_{H^{-1/2},H^{1/2}} = \langle M(E)f, g\rangle_{H^{1/2},H^{-1/2}} \quad \text{for all } f, g \in H^{-1/2}(\Gamma).$$

Now, let $(g, g') \in (\tilde{\ell}(E))^\circ$. For all $f \in H^{-1/2}(\Gamma)$, we have

$$0 = \tilde{\omega}((f, M(E)f), (g, g')) = \langle f, g' \rangle_{H^{-1/2}, H^{1/2}} - \langle M(E)f, g \rangle_{H^{1/2}, H^{-1/2}}.$$

Comparing with the previous line, this implies

$$\langle f, (g' - M(E)g) \rangle_{H^{-1/2}, H^{1/2}} = 0 \quad \text{for all } f \in H^{-1/2}(\Gamma).$$

hence $g' = M(E)g$, and $(g, g') \in \tilde{\ell}(E)$. So, $\tilde{\ell}(E) = (\tilde{\ell}(E))^\circ$ as wanted.

Case 2: E is an eigenvalue of $H_D^\sharp$. . We now prove the result when E is an isolated eigenvalue of $H_D^\sharp$ of finite multiplicity, that is $E \in \sigma(H_D^\sharp) \setminus \sigma_{\text{ess}}(H_D^\sharp)$. This case is novel to the best of our knowledge.

As before, we consider $\psi_E \in \widetilde{\mathcal{S}_E}$ and set $\widetilde{\text{Tr}}(\psi_E) = (f, f')$. We decompose ψ_E as $\psi_E = \psi_D + \psi_\Sigma$, and we get again

$$(H_D^\sharp - E)\psi_D = (E - \Sigma)\psi_\Sigma.$$

This time, the operator $(H_D^\sharp - E)$ is non-invertible. We consider the decomposition $L^2(\Omega^+) = K \oplus K^\perp$ with $K := \text{Ker}(H_D^\sharp - E)$. We deduce first that $\psi_\Sigma \in K^\perp$, and then that

$$\psi_D = (E - \Sigma)(H_D^\sharp - E)^\dagger \psi_\Sigma + \psi_K,$$

for some $\psi_K \in K$. Here, $(H_D^\sharp - E)^\dagger$ denotes the pseudo-inverse of $(H_D^\sharp - E)$. It is a bounded operator on $L^2(\Omega^+)$, as E is an isolated eigenvalue. Taking boundary trace shows that

$$f = \gamma^D \psi_\Sigma \quad \text{and} \quad f' = M(E)f + \gamma^N \psi_K,$$

with

$$M(E) := (E - \Sigma)\gamma^N (H_D^\sharp - E)^\dagger G_\Sigma.$$

We deduce that

$$\tilde{\ell}(E) \subset \{(f, M(E)f) \colon f \in \gamma^D K^\perp\} + \{(0, \gamma^N \psi_K) \colon \psi_K \in K\}.$$

Conversely, given $f \in \gamma^D K^\perp$ and $\psi_K \in K$, the function

$$\psi_\Sigma := (1 + (E - \Sigma)(H_D^\sharp - E)^\dagger) G_\Sigma f + \psi_K,$$

is in $\widetilde{\mathcal{S}_E}$ (we use here that $(H_D^\sharp - E)(H_D^\sharp - E)^\dagger = P_K^\perp$, where $P_K^\perp$ is the orthogonal projection on $K^\perp$, and that $G_\Sigma f$ is in $K^\perp$), and satisfies $\widetilde{\text{Tr}}(\psi_\Sigma) = (f, M(E)f) + (0, \gamma^N \Psi_K)$. So, we have the equality

$$\tilde{\ell}(E) = \{(f, M(E)f) \colon f \in \gamma^D K^\perp\} + \{(0, \gamma^N \psi_K) \colon \psi_K \in K\}.$$

From the isotropy of $\ell(E)$, we deduce that the operator $M(E)$ is symmetric on $\gamma^D K^\perp$, in the sense that

$$\langle f, M(E)g\rangle_{H^{-1/2},H^{1/2}} = \langle M(E)f, g\rangle_{H^{1/2},H^{-1/2}} \quad \text{for all } f, g \in \gamma^D K^\perp.$$

In addition, we also have

$$\langle f, \gamma^N \psi_K\rangle_{H^{-1/2},H^{1/2}} = 0 \quad \text{for all } f \in \gamma^D K^\perp,\ \psi_K \in K.$$

Since $\gamma^D K^\perp$ is of codimension $\dim(K)$ in $H^{-1/2}(\Gamma)$ while $\{\gamma^N \psi_K : \psi_K \in K\}$ is of dimension $\dim(K)$, we deduce that if $h \in H^{1/2}(\Gamma)$ satisfies $\langle f, h\rangle_{H^{-1/2},H^{1/2}} = 0$ for all $f \in \gamma^D K^\perp$, then $h = \gamma^N \psi_K$ for some $\psi_K \in K$.

Let us finally prove that $\tilde{\ell}(E)$ is Lagrangian. Let $(g, g') \in (\tilde{\ell}(E))^\circ$, and let $\psi_g \in \mathcal{D}^\sharp_{\max}$ be such that $\widetilde{\mathrm{Tr}}(\psi_g) = (g, g')$. We write $\psi_g = \psi_K + \psi_K^\perp$ with $\psi_K = P_K \psi_g$. Taking Dirichlet trace shows that $g = \gamma^D \psi_g = \gamma^D \psi_K^\perp \in \gamma^D K^\perp$. We set $h := g' - M(E)g$. We have, for all $f \in \gamma^D K^\perp$,

$$\begin{aligned} 0 &= \tilde{\omega}((f, M(E)f), (g, g')) \\ &= \langle f, g'\rangle_{H^{-1/2},H^{1/2}} - \langle M(E)f, g\rangle_{H^{1/2},H^{-1/2}} \\ &= \langle f, g' - M(E)g\rangle_{H^{-1/2},H^{1/2}} \\ &= \langle f, h\rangle_{H^{-1/2},H^{1/2}}. \end{aligned}$$

We deduce that $h = \gamma^D \psi_K'$ for some $\psi_K' \in K$, hence $g' = M(E)g + \gamma^D \psi_K'$. So, $(g, g') \in \tilde{\ell}(E)$, and $(\tilde{\ell}(E))^\circ = \tilde{\ell}(E)$ is Lagrangian. ■

4.5.4. Concluding remarks. The use of the boundary trace $\widetilde{\mathcal{H}_b}$ is suitable to study Schrödinger operators on the half-tubes Ω^+ or Ω^-. Indeed, one can detect that E is an eigenvalue for a general self-extension $(H^\sharp, \mathcal{D}^\sharp)$ as the crossing of the Lagrangian planes $\tilde{\ell}(E)$ and $\ell^\sharp$ in $\widetilde{\mathcal{H}_b}$. In addition, given a family of self-adjoint operators parametrized by $\ell_t^\sharp$, one can compute the spectral flow of this family as the Maslov index $\mathrm{Mas}(\tilde{\ell}(E), \ell_t^\sharp, \mathbb{T}^1)$. Since $(\widetilde{\mathcal{H}_b}, \tilde{\omega})$ satisfies Assumption B (hence Assumption A), this can be done using unitaries.

This setting is however not suitable to study the junction case, or more generally, to study operators on the whole tube Ω. The reason is the following. Let us consider the corresponding objects on the left tube Ω^-. The trace operators $\widetilde{\mathrm{Tr}}^-$ and $\widetilde{\mathrm{Tr}}^+$ depend on the left and right operators $H_D^{\sharp,-}$ and $H_D^{\sharp,+}$ respectively. In particular, they are unrelated! There is no analogue to Lemma 38 in this setting: the crossing of $\widetilde{\ell^+}(E)$ and $\widetilde{\ell^-}(E)$ does not imply that E is an eigenvalue of the bulk operator H. For instance, for $E = \Sigma$, we have $\widetilde{\ell^+}(\Sigma) = \widetilde{\ell^-}(\Sigma) = H^{-1/2}(\Gamma) \times \{0\}$, but Σ can be in the resolvent set of H. This is the reason why we chose to work in the $H^2(\Omega^\pm)$ setting, and to use the trace operator Tr.

Acknowledgements. We thank the anonymous referees for their comments and suggestions. We also thank the anonymous editor for pointing out an error in the initial version, and for the very interesting detailed comments and references on boundary triples.

Funding. This work was funded by the CNRS international cooperation tool PICS.

References

[1] V. I. Arnold, On a characteristic class entering into conditions of quantization. *Funkcional. Anal. i Priložen.* **1** (1967), 1–14; English transl., *Funct. Anal. Appl.* **1** (1967), 1–13 Zbl 0175.20303 MR 0211415

[2] M. F. Atiyah, V. K. Patodi, and I. M. Singer, Spectral asymmetry and Riemannian geometry. III. *Math. Proc. Cambridge Philos. Soc.* **79** (1976), no. 1, 71–99 Zbl 0325.58015 MR 397799

[3] J. C. Avila, H. Schulz-Baldes, and C. Villegas-Blas, Topological invariants of edge states for periodic two-dimensional models. *Math. Phys. Anal. Geom.* **16** (2013), no. 2, 137–170 Zbl 1271.81210 MR 3063955

[4] J. Behrndt, S. Hassi, and H. de Snoo, *Boundary value problems, Weyl functions, and differential operators*. Monographs in Mathematics 108, Birkhäuser/Springer, 2020 Zbl 1457.47001 MR 3971207

[5] J. Behrndt and M. Langer, Boundary value problems for elliptic partial differential operators on bounded domains. *J. Funct. Anal.* **243** (2007), no. 2, 536–565 Zbl 1132.47038 MR 2289696

[6] J. Behrndt and T. Micheler, Elliptic differential operators on Lipschitz domains and abstract boundary value problems. *J. Funct. Anal.* **267** (2014), no. 10, 3657–3709 Zbl 1300.35026 MR 3266243

[7] B. Booss-Bavnbek and K. Furutani, The Maslov index: a functional analytical definition and the spectral flow formula. *Tokyo J. Math.* **21** (1998), no. 1, 1–34 Zbl 0932.37063 MR 1630119

[8] B. Booß-Bavnbek and C. Zhu, The Maslov index in weak symplectic functional analysis. *Ann. Global Anal. Geom.* **44** (2013), no. 3, 283–318 Zbl 1307.53063 MR 3101860

[9] G. Bräunlich, G. M. Graf, and G. Ortelli, Equivalence of topological and scattering approaches to quantum pumping. *Comm. Math. Phys.* **295** (2010), no. 1, 243–259 Zbl 1227.34089 MR 2585997

[10] G. Carron, Déterminant relatif et la fonction Xi. *Amer. J. Math.* **124** (2002), no. 2, 307–352 Zbl 1014.34015 MR 1890995

[11] G. Cox, C. K. R. T. Jones, and J. L. Marzuola, A Morse index theorem for elliptic operators on bounded domains. *Comm. Partial Differential Equations* **40** (2015), no. 8, 1467–1497 Zbl 1335.35166

[12] S. De Bièvre and J. V. Pulé, Propagating edge states for a magnetic Hamiltonian. *Math. Phys. Electron. J.* **5** (1999), article no. 3 Zbl 0930.35144 MR 1703586

[13] J. Deng and C. Jones, Multi-dimensional Morse index theorems and a symplectic view of elliptic boundary value problems. *Trans. Amer. Math. Soc.* **363** (2011), no. 3, 1487–1508 Zbl 1210.35056 MR 2737274

[14] J. Deng and S. Nii, Infinite-dimensional Evans function theory for elliptic eigenvalue problems in a channel. *J. Differential Equations* **225** (2006), no. 1, 57–89 Zbl 1115.35091 MR 2228692

[15] J. Deng and S. Nii, An infinite-dimensional Evans function theory for elliptic boundary value problems. *J. Differential Equations* **244** (2008), no. 4, 753–765 MR 2391343

[16] A. Drouot, The bulk-edge correspondence for continuous dislocated systems. *Ann. Inst. Fourier (Grenoble)* **71** (2021), no. 3, 1185–1239 Zbl 1492.81054 MR 4398223

[17] N. Dunford and J. T. Schwartz, *Linear operators.* Part II: Spectral theory. Self adjoint operators in Hilbert space. Interscience Publishers, New York and London, 1963 Zbl 0128.34803 MR 0188745

[18] K. Furutani, Fredholm–Lagrangian–Grassmannian and the Maslov index. *J. Geom. Phys.* **51** (2004), no. 3, 269–331 Zbl 1076.53100 MR 2079414

[19] D. Gilbarg and N. Trudinger, Elliptic partial differential equations of second order Classics in Mathematics. Springer, Berlin, 2001 Zbl 1042.35002 MR 1814364

[20] D. Gontier, Edge states in ordinary differential equations for dislocations. *J. Math. Phys.* **61** (2020), no. 4, article no. 043507 Zbl 1443.81030 MR 4090721

[21] D. Gontier, Spectral properties of periodic systems cut at an angle. *C. R. Math. Acad. Sci. Paris* **359** (2021), 949–958 Zbl 07410661 MR 4322996

[22] G. M. Graf and M. Porta, Bulk-edge correspondence for two-dimensional topological insulators. *Comm. Math. Phys.* **324** (2013), no. 3, 851–895 Zbl 1291.82120 MR 3123539

[23] G. Grubb, A characterization of the non-local boundary value problems associated with an elliptic operator. *Ann. Scuola Norm. Sup. Pisa Cl. Sci. (3)* **22** (1968), 425–513 Zbl 0182.14501 MR 239269

[24] Y. Hatsugai, Chern number and edge states in the integer quantum Hall effect. *Phys. Rev. Lett.* **71** (1993), no. 22, 3697–3700 Zbl 0972.81712 MR 1246070

[25] Y. Hatsugai, Edge states in the integer quantum Hall effect and the Riemann surface of the Bloch function. *Phys. Rev. B* **48** (1993), no. 16, 11851–11862

[26] R. Hempel and M. Kohlmann, A variational approach to dislocation problems for periodic Schrödinger operators. *J. Math. Anal. Appl.* **381** (2011), no. 1, 166–178 Zbl 1220.35028 MR 2796200

[27] R. Hempel and M. Kohlmann, Dislocation problems for periodic Schrödinger operators and mathematical aspects of small angle grain boundaries. In *Spectral theory, mathematical system theory, evolution equations, differential and difference equations*, pp. 421–432, Oper. Theory Adv. Appl. 221, Birkhäuser/Springer Basel AG, Basel, 2012 Zbl 1256.35013 MR 2954079

[28] P. Howard, Y. Latushkin, and A. Sukhtayev, The Maslov index for Lagrangian pairs on $\mathbb{R}^{2n}$. *J. Math. Anal. Appl.* **451** (2017), no. 2, 794–821 Zbl 1377.35073 MR 3624767

[29] P. Howard, Y. Latushkin, and A. Sukhtayev, The Maslov and Morse indices for system Schrödinger operators on $\mathbb{R}$. *Indiana Univ. Math. J.* **67** (2018), no. 5, 1765–1815 Zbl 1408.53106 MR 3875243

[30] P. Howard and A. Sukhtayev, The Maslov and Morse indices for Schrödinger operators on [0, 1]. *J. Differential Equations* **260** (2016), no. 5, 4499–4549 Zbl 1337.47064 MR 3437596

[31] T. Kato, *Perturbation theory for linear operators*. Grundlehren Math. Wiss. 132, Springer, New York, 1966 Zbl 0148.12601 MR 0203473

[32] V. Kostrykin and R. Schrader, Kirchhoff's rule for quantum wires. *J. Phys. A* **32** (1999), no. 4, 595–630 Zbl 0928.34066 MR 1671833

[33] Y. Latushkin and S. Sukhtaiev, The Maslov index and the spectra of second order elliptic operators. *Adv. Math.* **329** (2018), 422–486 Zbl 06863449 MR 3783419

[34] J. Leray, Analyse lagrangienne et mécanique quantique. In *Séminaire sur les équations aux Dérivées Partielles (1976–1977),* I, Exp. No. 1, Collège de France, Paris, 1977 MR 0501198

[35] V. B. Lidskii, On the number of solutions with integrable square of the system of differential equations $-y'' + P(t)y = \lambda y$. *Doklady Akad. Nauk SSSR (N.S.)* **95** (1954), 217–220 Zbl 0058.31402 MR 0062297

[36] J.-L. Lions and E. Magenes, *Non-homogeneous boundary value problems and applications. Vol. I.* Grundlehren Math. Wiss. 181, Springer, Berlin etc., 1972 Zbl 0223.35039 MR 0350177

[37] V. Maslov, V. Bouslaev, and V. Arnol'd, *Théorie des perturbations et méthodes asymptotiques.* Dunod, Paris, 1972 Zbl 0247.47010

[38] J. Phillips, Self-adjoint Fredholm operators and spectral flow. *Canad. Math. Bull.* **39** (1996), no. 4, 460–467 Zbl 0878.19001 MR 1426691

[39] M. Reed and B. Simon, *Methods of modern mathematical physics.* II. Fourier analysis, self-adjointness. Academic Press, New York and London, 1975 Zbl 0308.47002 MR 0493420

[40] M. Reed and B. Simon, *Methods of modern mathematical physics.* IV. Analysis of operators. Academic Press, New York and London, 1978 Zbl 0401.47001 MR 0493421

[41] M. Reed and B. Simon, *Methods of modern mathematical physics.* III. Scattering theory. Academic Press, New York and London, 1979 Zbl 0405.47007 MR 0529429

[42] D. J. Thouless, Quantization of particle transport. *Phys. Rev. B (3)* **27** (1983), no. 10, 6083–6087 MR 704595

[43] J. v. Neumann, Allgemeine Eigenwerttheorie Hermitescher Funktionaloperatoren. *Math. Ann.* **102** (1930), no. 1, 49–131 JFM 55.0824.02 MR 1512569

[44] M. I. Višik, On general boundary problems for elliptic differential equations. *Trudy Moskov. Mat. Obšč.* **1** (1952), 187–246; English transl., *Amer. Math. Soc. Transl. (2)* **24** (1963), 107–172 Zbl 0047.09502 MR 0051404

[45] N. Waterstraat, Fredholm operators and spectral flow. *Rend. Semin. Mat. Univ. Politec. Torino* **75** (2017), no. 1, 7–51 Zbl 07236744 MR 3835757

[46] H. Weyl, Über gewöhnliche Differentialgleichungen mit Singularitäten und die zugehörigen Entwicklungen willkürlicher Funktionen. *Math. Ann.* **68** (1910), no. 2, 220–269 Zbl 41.0343.01 MR 1511560

Received 30 January 2021; revised 18 February 2022.

David Gontier
CEREMADE, University of Paris-Dauphine, PSL University, 75016 Paris, France;
gontier@ceremade.dauphine.fr