Spectra of graphene nanoribbons with armchair and zigzag boundary conditions

SPECTRA OF GRAPHENE NANORIBBONS WITH ARMCHAIR AND ZIGZAG BOUNDARY CONDITIONS

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Abstract. We study the spectral properties of the two-dimensional Dirac operator on bounded domains together with the appropriate boundary conditions which provide a (continuous) model for graphene nanoribbons. These are of two types, namely the so–called armchair and zigzag boundary conditions, depending on the line along which the material was cut. In the former case, we show that the spectrum behaves in what might be called a *classical way*, while in the latter we prove the existence of a sequence of finite multiplicity eigenvalues converging to zero and which correspond to edge states.

1. Introduction

The Dirac operator in two–dimensional Euclidean space has received much attention in the literature recently, partly due to its connection to the study of graphene [3, 1, 22, 17], partly due to the interesting spectral properties in its own right [8, 7, 23]. One key ingredient in both situations is the behaviour with respect to boundary conditions, in the case where the domain considered is not the whole space. On the one hand, and due to the scale of graphene–based devices, the way in which the hexagonal lattice is cut affects the behaviour of the material and has to be taken into consideration. On the other hand, this poses some issues regarding the appropriate boundary conditions that should be imposed on the Dirac operator.

In a previous paper on the subject [23], Schmidt showed that for bounded domains in $\mathbb{R}^2$ imposing a vanishing condition on the boundary for one of the components of the vector of eigenfunctions would imply that zero would be an eigenvalue of infinity multiplicity and thus the essential spectrum would be non-empty. This effect is a consequence of the fact that, in the functional setting considered in [23], as long as the other function in the eigenvector is analytic in the domain under consideration, then this will be in the kernel of the operator, as this second function will satisfy the necessary Cauchy–Riemann equations. Although in Schmidt's example the square of each of the remaining eigenvalues was an eigenvalue (of finite multiplicity) of the Dirichlet Laplacian on the same domain, it is known that, at least for balls in three dimensional space, the addition of a potential may *destabilize* the zero eigenvalue and give rise to an infinite sequence of eigenvalues converging to zero [8].

The purpose of the present paper is to show that a similar effect may occur without the presence of a potential, as a result of imposing appropriate boundary

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conditions. Furthermore, these boundary conditions occur in a natural way in the case of graphene as a consequence of the boundary effect of the hexagonal lattice referred to above.

Several remarks are in order here. On the one hand, there are examples in the physics literature where such sequences may be found, although the existence of the sequence in not always mentioned explicitly and only some states are presented [3, 26]. In spite of this, and as far as we are aware, there has been no rigorous mathematical study of this effect. Although, as stated in the Schmidt paper mentioned above, the boundary conditions considered there are "essentially the only type of local boundary condition which gives rise to a self-adjoint Dirac operator," later in the paper (page 511) the assumption that the zero boundary condition is taken only by the first component of the eigenvector is made. It is also stated that the "mixed boundary conditions where both types are employed at different parts of $\partial\Omega$" will not be considered. In fact, it is precisely this type of mixed boundary condition that will cause the eigenvalue of infinite multiplicity to split into an infinite sequence of eigenvalues with finite multiplicities. We thus see, for example, that an annulus with what is known in the literature as *zigzag* boundary conditions yields a sequence of eigenvalues converging to zero, with the corresponding eigenfunctions localizing near the outer boundary of the annulus – see the example in Section 4.2. The existence of such a sequence is a general feature of the zigzag boundary conditions and is reflected in non-empty essential spectrum (containing zero) and the fact that the norm of the associated eigenfunctions, called edge states in the physics literature, tends to zero in any compact subset of the domain considered as the corresponding energy approaches zero. Furthermore, we observe that for the explicit examples with zigzag boundary conditions considered in Section 4, the eigenvalues in this sequence approach zero exponentially.

At the same time, these results raise the question of which of these eigenvalues and eigenfunctions are physically relevant, taking into account the dimensions of the domain and the fact that as the sequence of eigenvalues approaches zero, the number of oscillations in the eigenfunctions approaches infinity. It is well known from the physics literature that graphene can be described by Dirac's equation only for sufficiently low energies and long wavelengths – see *e.g.* [1].

Besides models defined on bounded domains, we also consider infinite strips (waveguides), for which we obtain some preliminary results. In the case of armchair boundary conditions, where only straight strips seem to be physically relevant *cf.* [1], we see that there is a gap in the essential spectrum (depending on a physical parameter) without any eigenvalues in that gap. In the case of zigzag boundary conditions used to describe curved waveguides we see that the essential spectrum covers the whole real line.

The plan of the paper is as follows. In the next section, we lay out the basic concepts related to the Hamiltonian and the two different types of boundary conditions. The corresponding spectral properties which are the main results of the paper are studied in Section 3. These results are then illustrated by examples for which the spectrum may be computed explicitly and which are presented in Section 4. A further example for an infinite strip (waveguide) is given in Section 5 and the results presented are discussed in the last section.

2. Hamiltonians and boundary conditions

Graphene is a two dimensional planar sheet of carbon atoms organized in a honeycomb crystal lattice as shown in Figure 1, which, when cut into a strip, is called a graphene nanoribbon. One of the first theoretical studies of such systems, and particularly the existence of edge states, can be found in [10]. The continuous model for nanoribbons is a two dimensional Dirac operator

$$H := \begin{pmatrix} 0 & \tau^* & 0 & 0 \\ \tau & 0 & 0 & 0 \\ 0 & 0 & 0 & -\tau \\ 0 & 0 & -\tau^* & 0 \end{pmatrix}, \tag{1}$$

where $\tau := -i\partial_1 + \partial_2$ and τ^* is the formal adjoint, *i.e.* $\tau^* := -i\partial_1 - \partial_2$, see *e.g.* [3, 1] for details. The hamiltonian H acts in $L^2(\Omega, \mathbb{C}^4)$, $\Omega \subset \mathbb{R}^2$, *i.e.* on vector valued functions, often called spinors. In what follows, we use H to denote a differential expression only and we will introduce different notations for the corresponding self-adjoint operators obtained by restricting it to different function spaces.

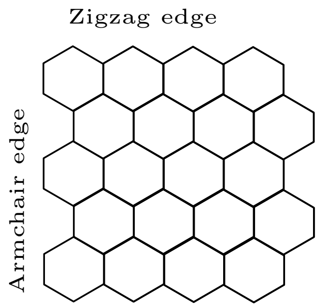

FIGURE 1. Sheet of graphene

The orientation of the strip in a graphene sheet, *i.e.* the way how the strip is cut out from the plane, is essential for the physical properties of graphene nanoribbons. This is reflected in the type of boundary conditions that is imposed giving rise to two standard choices, the so-called zigzag and armchair boundary conditions, the names corresponding to the shape of the edge of the strip, as illustrated in Figure 1. Note that there are other armchair directions besides the vertical one.

We fix the horizontal direction x_1 to be parallel to the zigzag edge and the vertical x_2 to the armchair edge and consider two infinite straight strips Ω_i $(i = 1, 2)$ in the x_1 and x_2 directions respectively; more precisely $\Omega_1 := \mathbb{R} \times (-b, b)$ and $\Omega_2 := (-a, a) \times \mathbb{R}$. In this setting the boundary conditions, imposed on the components of the spinor $\Psi = (\Psi_1, \Psi_2, \Psi_3, \Psi_4)$, read

$$\text{zigzag}: \quad \Psi_i(x_1, -b) = 0, \ \Psi_{i+1}(x_1, b) = 0, \ (i = 1, 3), \ \forall x_1 \in \mathbb{R}, \tag{2}$$

$$\text{armchair}: \quad \Psi_j(-a, x_2) = \Psi_{j+2}(-a, x_2), \tag{3}$$

$$\Psi_j(a, x_2) = e^{\mathrm{i}\Theta} \Psi_{j+2}(a, x_2), \ (j = 1, 2), \ \forall x_2 \in \mathbb{R}, \ \Theta \in \mathbb{R}, \tag{4}$$

where Θ is a physical parameter related to the number of unit cells of atoms in the x_1 direction in the strip (see *e.g.* [3]). It it possible to argue that zigzag boundary conditions are appropriate even when considering domains whose sides are not parallel to the zigzag edge described above [1]. More precisely, to model graphene nanoribbons, zigzag boundary conditions should be imposed except for straight parts of the boundary in specific directions that are described by armchair boundary conditions.

These two boundary conditions clearly have different natures, to which there will correspond different spectral behaviour. More precisely, while zigzag conditions enable us to separate the first two components of the spinor from the last pair, armchair conditions connect its odd and even components. More important, there is a substantial difference in the domains of definition of the corresponding Hamiltonians depending on whether zigzag or armchair boundary conditions are being imposed.

2.1. **Armchair boundary conditions.** We describe the armchair case first, as this leads to a "standard" problem. To do this, let's define the symmetric operator $\dot{H}_{\rm ac}$ by

$$\begin{aligned} &\dot{H}_{\rm ac}\Psi := H\Psi \\ &\operatorname{Dom}(\dot{H}_{\rm ac}) := \left\{\Psi \in C^\infty(\overline{\Omega}_2, \mathbb{C}^4) : \Psi \text{ satisfies (3) and } (4), H\Psi \in L^2(\Omega, \mathbb{C}^4)\right\}. \end{aligned} \tag{5}$$

Using integration by parts we obtain

$$\|\dot{H}_{\rm ac}\Psi\|^2 + \|\Psi\|^2 = \|\partial_1\Psi\|^2 + \|\partial_2\Psi\|^2 + \|\Psi\|^2, \tag{6}$$

i.e. the graph norm of $\dot{H}_{\rm ac}$ is the Sobolev space norm. We denote $H_{\rm ac}$ the closure of $\dot{H}_{\rm ac}$ and describe its domain and adjoint in details.

Proposition 1.

$$\begin{aligned} &H_{\rm ac}\Psi = H\Psi, \\ &\operatorname{Dom}(H_{\rm ac}) = \big\{\Psi \in W^{1,2}(\Omega_2, \mathbb{C}^4) : \Psi \text{ satisfies (3) and (4)} \\ &\qquad\qquad \text{in the sense of traces}\big\}, \end{aligned} \tag{7}$$

and $H_{\rm ac}$ is self-adjoint.

Proof. We give a sketch of the proof only. The domain of the closure of $\dot{H}_{\rm ac}$ can be obtained immediately from the expression for the graph norm (6).

One possible way how to prove self-adjointness of $H_{\rm ac}$ is to show that $H_{\rm ac}^2$ is self-adjoint and use the identity $H_{\rm ac}^2 - \mathrm{i} = (H_{\rm ac} - \sqrt{\mathrm{i}})(H_{\rm ac} + \sqrt{\mathrm{i}})$, particularly $\operatorname{Ran}(H_{\rm ac}^2 - \mathrm{i}) \subset \operatorname{Ran}(H_{\rm ac} - \sqrt{\mathrm{i}})$, together with the basic criterion of self-adjointness [21, Thm.VII.3]. The self-adjointness of $H_{\rm ac}^2$ can be justified as follows. Using a standard approach relying on the difference quotients and the elliptic regularity [6, Chap.5.8.2., Chap.6.3.], we can show that $H_{\rm ac}^2 = \operatorname{diag}\{-\Delta, -\Delta, -\Delta, -\Delta\}$, acting on spinors Ψ from $W^{2,2}(\Omega_1, \mathbb{C}^4)$ such that Ψ and $H_{\rm ac}\Psi$ satisfy boundary conditions (3)-(4), is associated via the representation theorem [16] to the quadratic form $h_{\rm ac}[\Psi] := \|H_{\rm ac}\Psi\|^2$. □

We remark that if instead of the infinite strip Ω_2 we consider a finite rectangle $(-a, a) \times (-b, b)$, complementing the armchair boundary conditions with periodic boundary conditions on the horizontal parts of the boundary ($x_2 = \pm b$), using similar arguments as above defines a self-adjoint operator acting on $W^{1,2}$ functions satisfying these boundary conditions.

2.2. **Zigzag boundary conditions.** Zigzag boundary conditions are quite different from the armchair case considered in the previous section. If we were to proceed in an analogous way to (5), with a symmetric operator acting as H defined on smooth functions satisfying the boundary conditions (2), we would then conclude that the graph norm cannot be written as a $W^{1,2}$ norm. Since zigzag boundary conditions are physically relevant also on the non-straight parts of the boundary, we shall consider a general bounded domain $\Omega \subset \mathbb{R}^2$ with the technical assumptions on Ω being stated in specific results. Some claims about the domain of definition and supersymmetry are relevant also in the case of the infinite strip Ω_1 and its curved (non self-intersecting) version – see Section 5.

Due to the nature of the boundary conditions, we can split the 4×4 Hamiltonian H into two 2×2 subsystems with a similar structure, namely

$$H_1 := \begin{pmatrix} 0 & \tau^* \\ \tau & 0 \end{pmatrix}, \quad H_2 := \begin{pmatrix} 0 & -\tau \\ -\tau^* & 0 \end{pmatrix}. \tag{8}$$

In what follows we will obtain a self-adjoint realization of H_1 in $L^2(\Omega, \mathbb{C}^2)$. Zigzag boundary conditions correspond to Dirichlet boundary conditions for the components of the spinor and the case of $\Psi_1 = 0$ at $\partial\Omega$ was already analysed extensively in [23]. Here we concentrate on two more general cases, illustrated in Figure 2, that were not considered in that article.

In the first, $\partial\Omega$ is assumed to have two connected components $\partial\Omega^i$ $(i = 1, 2)$, *i.e.* $\partial\Omega = \partial\Omega^1 \cup \partial\Omega^2$, a typical example of which is an annulus, where $\partial\Omega^i$ are the inner $(i = 1)$ and the outer circles $(i = 2)$. We impose "complementary" Dirichlet boundary conditions for each of the spinor components on the different part of the boundary, *i.e.* $\Psi_i = 0$ at $\partial\Omega^i$. The corresponding closed realization of the differential expression will be denoted by A.

In the second, $\partial\Omega$ is assumed to be connected and divided by two points p_1 and p_2 in $\partial\Omega$ into two (open) pieces $\partial\Omega_1$ and $\partial\Omega_2$, *i.e.* $\partial\Omega = \partial\Omega_1 \cup \partial\Omega_2 \cup \{p_1, p_2\}$. We then impose the "interchanging" Dirichlet boundary conditions for the spinor components, *i.e.* $\Psi_i = 0$ at $\partial\Omega_i$. The closed realization of τ will be denoted by B. We remark that more general situations like any finite number of connected components of $\partial\Omega$ or dividing points or a combination of both can be studied in a similar way with the proofs given here being generalized in a straightforward fashion.

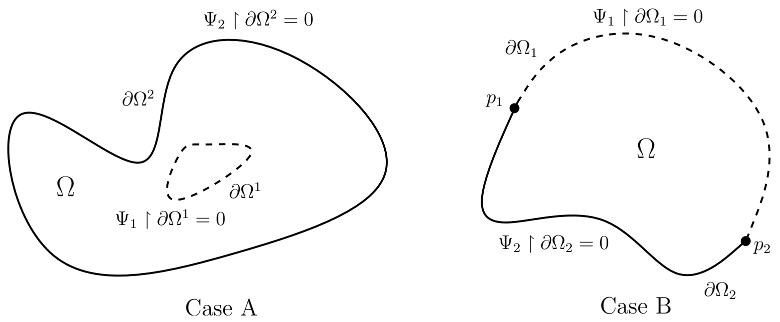

FIGURE 2. Two cases of domains and boundary conditions.

H_1 has a formal supersymmetric structure, *cf.* [24, Chap.5], therefore when we find a densely defined and closed realization $T = A, B$ of τ, then

$$H_{zz} \equiv H_{zz}^T := \begin{pmatrix} 0 & T^* \\ T & 0 \end{pmatrix} \tag{9}$$

is self-adjoint, *cf.* [24, Lem.5.3]. The supersymmetric structure of H_{zz}^T, *i.e.* T^*T and TT^* are so-called supersymmetric partners, immediately yields also the quadratic forms associated to T^*T and TT^* and the relation between spectra of these two operators.

Proposition 2. *Let T be densely defined and closed. T^*T, TT^* are associated with the closed symmetric quadratic forms $t_{T^*T}[\psi] := \|T\psi\|^2$, $t_{TT^*}[\psi] := \|T^*\psi\|^2$ defined on* $\mathrm{Dom}\,(T)$, $\mathrm{Dom}\,(T^*)$, *respectively. Moreover,* $\sigma(TT^*) \cup \{0\} = \sigma(T^*T) \cup \{0\}$.

Proof. The proof can be found in [16, VI.2.1] and [24, Cor.5.6]. □

We focus mainly on the spectrum of $H_{zz}^2 = \mathrm{diag}(T^*T, TT^*)$. Both T^*T and TT^* act as Laplacians locally in Ω and they represent a realization of Laplacians with the combination of Dirichlet and "Cauchy-Riemann" or "anti-Cauchy-Riemann" boundary conditions.

The initial step for the spectral analysis is showing the existence of a closed realization of τ and the description of its domain as well as the domain of the adjoint operator. In the first situation, *i.e.* the boundary of Ω is made up of two connected components, we give a full description of both domains. In the second one, *i.e.* the connected boundary is divided into two parts, we start with a closable realization of τ and find the domain of the adjoint. In this case, and although we were not able to fully determine the domain of the closure of τ, we can provide useful inclusions from both sides.

Proposition 3. *Let Ω be a bounded connected domain with a locally Lipschitz boundary $\partial\Omega$ that is made up of two nonempty connected components $\partial\Omega^i$ $(i=1,2)$ with $\operatorname{dist}(\partial\Omega^1,\partial\Omega^2)>0$. Let A be the operator acting as $A\psi:=\tau\psi$ on the domain*

$$\operatorname{Dom}(A) := \{\psi \in L^2(\Omega)\cap W^{1,2}_{\mathrm{loc}}(\Omega\cup\partial\Omega^1) : \psi\restriction\partial\Omega^1 = 0,\ \tau\psi\in L^2(\Omega)\}, \tag{10}$$

where $W^{1,2}_{\mathrm{loc}}(\Omega\cup\partial\Omega^1)$ means the functions from $W^{1,2}(\Omega')$ for any $\Omega'\subset\Omega$, $\overline{\Omega'}\subset\Omega\cup\partial\Omega^1$.

Then A is closed and A^* acts as $A^*\phi:=\tau^*\phi$ on the domain

$$\operatorname{Dom}(A^*) := \{\phi \in L^2(\Omega)\cap W^{1,2}_{\mathrm{loc}}(\Omega\cup\partial\Omega^2) : \phi\restriction\partial\Omega^2 = 0,\ \tau^*\phi\in L^2(\Omega)\}, \tag{11}$$

where $W^{1,2}_{\mathrm{loc}}(\Omega\cup\partial\Omega^2)$ is introduced in an analogous way.

Proof. The proof is a modification of that given in [23, Prop.1].

Denote by $\mathscr{D}^*$ the set on the right hand side of (11). We first show that $\mathscr{D}^*\subset\operatorname{Dom}(A^*)$.

Take $\phi\in\mathscr{D}^*$ and $\psi\in\operatorname{Dom}(A)$. Let $\Gamma\subset\Omega$ be a closed curve that divides Ω into two subdomains with a locally Lipschitz boundary $\tilde\Omega^i$ $(i=1,2)$, *i.e.* $\Omega=\tilde\Omega^1\cup\tilde\Omega^2\cup\Gamma$, such that $\partial\tilde\Omega^i=\partial\Omega^i\cup\Gamma$ and $\operatorname{dist}(\Gamma,\partial\Omega^i)>0$. The restriction of ϕ to $\tilde\Omega^2$ belongs to $W^{1,2}(\tilde\Omega^2)$ and satisfies Dirichlet boundary conditions on $\partial\Omega^2$; a similar fact holds for $\psi\in\operatorname{Dom}(A)$ restricted to $\tilde\Omega^1$. Therefore ψ and ϕ can be approximated in the $W^{1,2}$ norm in $\tilde\Omega^1$ and $\tilde\Omega^2$, by smooth functions ψ_n and ϕ_n whose support does not intersect $\partial\Omega^1$ and $\partial\Omega^2$, respectively. Then

$$\int_\Omega \overline{\phi}A\psi = \lim_{n\to\infty}\int_{\tilde\Omega^1}\overline{\phi}\tau\psi_n + \lim_{n\to\infty}\int_{\tilde\Omega^2}\overline{\phi_n}\tau\psi = \int_\Omega\overline{(\tau^*\phi)}\psi, \tag{12}$$

where we used Gauss's theorem and the fact that boundary terms vanish on $\partial\Omega^i$ and cancel (in the limit) on Γ.

For the inclusion in the other direction, *i.e.* $\mathscr{D}^*\supset\operatorname{Dom}(A^*)$, we consider an operator $A_0\subset A$ defined on

$$\operatorname{Dom}(A_0) := \{\psi\in C^\infty(\overline{\Omega}) : \operatorname{supp}\psi\cap\partial\Omega^1=\emptyset\}.$$

and we prove the second inclusion in $\operatorname{Dom}(A^*)\subset\operatorname{Dom}(A_0^*)\subset\mathscr{D}^*$. Let $\phi\in\operatorname{Dom}(A_0^*)$, $\eta:=A_0^*\phi$ and $\psi\in\operatorname{Dom}(A_0)$. Let further K be a compact subset of $\Omega\cup\partial\Omega^2$ and $\chi\in C_0^\infty(\mathbb{R}^2)$ a real function such that $\operatorname{supp}\ \chi\cap\partial\Omega^1=\emptyset$ and $\chi\restriction K=1$. We take positive ε and mollify $\chi\phi$ and $\chi\eta$, that is, we consider a convolution $J_\varepsilon:=\cdot * j_\varepsilon$ with the real function $j_\varepsilon\in C_0^\infty(B_\varepsilon)$ and write $\phi_\varepsilon:=J_\varepsilon(\chi\phi)$ and $\eta_\varepsilon:=J_\varepsilon(\chi\eta)$. For an arbitrary $\varphi\in C_0^\infty(\mathbb{R}^2)$ we then have

$$\begin{aligned}\int_{\mathbb{R}^2}\varphi\overline{\eta_\varepsilon} &= \int_{\mathbb{R}^2}\chi J_\varepsilon(\varphi)\overline{A_0^*\phi} = \int_{\mathbb{R}^2}\tau(\chi J_\varepsilon(\varphi))\overline{\phi}\\ &= \int_{\mathbb{R}^2}\left(J_\varepsilon(\varphi)\tau(\chi)+\chi\tau(J_\varepsilon(\varphi))\right)\overline{\phi} = \int_{\mathbb{R}^2}\varphi J_\varepsilon(\tau(\chi)\overline{\phi})+\tau(\varphi)J_\varepsilon(\chi\overline{\phi})\\ &= \int_{\mathbb{R}^2}\varphi\left(J_\varepsilon(\tau(\chi)\overline{\phi})-\tau(J_\varepsilon(\chi\overline{\phi}))\right) = \int_{\mathbb{R}^2}\varphi\overline{(-J_\varepsilon(\tau^*(\chi)\phi)+\tau^*\phi_\varepsilon)},\end{aligned} \tag{13}$$

where we used integration by parts, the fact that $\tau^*=-\overline{\tau}$, commutation of mollification with the derivative for smooth functions, and the fact that $\chi J_\varepsilon(\varphi)\restriction\Omega\in\operatorname{Dom}(A_0)$ in the second equality. Therefore $\tau^*\phi_\varepsilon=\eta_\varepsilon+J_\varepsilon(\tau^*(\chi)\phi)$ in $L^2(\mathbb{R}^2)$ and integration by parts yields

$$\int_{\mathbb{R}^2}|\tau^*\phi_\varepsilon-\tau^*\phi_\delta|^2 = \int_{\mathbb{R}^2}|\partial_1\phi_\varepsilon-\partial_1\phi_\delta|^2+|\partial_2\phi_\varepsilon-\partial_2\phi_\delta|^2 \tag{14}$$

for $\varepsilon, \delta > 0$. Hence,

$$\|\partial_i \phi_\varepsilon - \partial_i \phi_\delta\|_{L^2(\mathbb{R}^2)} \leq \|\eta_\varepsilon - \eta_\delta\|_{L^2(\mathbb{R}^2)} + \|J_\varepsilon(\tau^*(\chi)\phi) - J_\delta(\tau^*(\chi)\phi)\|_{L^2(\mathbb{R}^2)} \tag{15}$$

and therefore $\partial_i \phi_\varepsilon$ converges to $\phi^{(i)}$ in $L^2(\mathbb{R}^2)$. Thus, for arbitrary $\varphi \in C_0^\infty(\mathbb{R}^2)$ we have

$$-\int_{\mathbb{R}^2} \phi^{(i)} \varphi = \lim_{\epsilon \to 0} \int_{\mathbb{R}^2} J_\varepsilon(\chi\phi)\partial_i \varphi = \int_{\mathbb{R}^2} \chi\phi\partial_i\varphi, \tag{16}$$

Hence, if we take an arbitrary open $\Omega' \subset \Omega$ such that $\overline{\Omega'} \subset \Omega \cup \partial\Omega^2$ and consider $K := \overline{\Omega'}$, we get that $\phi \in W^{1,2}(\Omega')$, since $\phi^{(i)}$ are in fact the weak derivatives of ϕ when $\operatorname{supp}\varphi \subset \Omega'$.

On any compact subset of Ω, we have

$$\tau^*\phi = -\mathrm{i}\phi^{(1)} - \phi^{(2)} = \lim_{\varepsilon \to 0} \tau^*\phi_\varepsilon = A_0^*\phi \tag{17}$$

and Gauss's theorem yields for every $\psi \in \operatorname{Dom}(A_0)$

$$0 = \langle \phi, A_0\psi\rangle - \langle A_0^*\phi, \psi\rangle = \langle \phi, \tau\psi\rangle - \langle \tau^*\phi, \psi\rangle = \int_{\partial\Omega^2} (-\mathrm{i}n_1 + n_2)\psi \operatorname{Tr}\overline{\phi}, \tag{18}$$

where $\vec{n}$ is the outward pointing unit normal vector to $\partial\Omega^2$. Therefore $\phi \restriction \partial\Omega^2$ vanishes and thus $\operatorname{Dom}(A_0^*) \subset \mathscr{D}^*$.

If we repeat the described procedure for A^*, we obtain $A^{**} = \overline{A} = A$. $\square$

Proposition 4. *Let Ω be a bounded connected domain with locally Lipschitz and connected boundary $\partial\Omega$. Let further $p_i \in \partial\Omega$ $(i = 1, 2)$ be two distinct points dividing the boundary into two (non-empty and open) parts such that $\partial\Omega = \partial\Omega_1 \cup \partial\Omega_2 \cup \{p_1, p_2\}$. If B_0 is an operator acting as τ on the domain*

$$\begin{aligned} \operatorname{Dom}(B_0) := \{\psi \in C^\infty(\Omega) : \exists\psi_0 \in C_0^\infty(\mathbb{R}^2), \psi = \psi_0 \restriction \Omega, \\ \operatorname{supp}\psi \cap \overline{\partial\Omega_1} = \emptyset\}, \end{aligned} \tag{19}$$

then B_0 is closable and

$$\mathscr{D}_0 + \mathscr{D}_{\mathrm{loc}} \subset \operatorname{Dom}(B) \subset \mathscr{D}, \tag{20}$$

where

$$\mathscr{D}_0 := \{\psi_1 \in W^{1,2}(\Omega) : \psi_1 \restriction \partial\Omega_1 = 0\},$$

$$\begin{aligned} \mathscr{D}_{\mathrm{loc}} := \{\psi_2 \in L^2(\Omega) \cap W^{1,2}_{\mathrm{loc}}(\Omega \cup \partial\Omega_1) : \\ \exists U_i \subset \mathbb{R}^2 \ (i = 1, 2) \text{ open neighborhoods of } p_i \ (i = 1, 2), \text{ respectively}, \\ \psi_2 \restriction U_{1,2} = 0, \tau\psi_2 \in L^2(\Omega)\}, \end{aligned}$$

and

$$\mathscr{D} := \{\psi \in L^2(\Omega) \cap W^{1,2}_{\mathrm{loc}}(\Omega \cup \partial\Omega_1) : \psi \restriction \partial\Omega_1 = 0 \text{ a.e.}, \tau\psi \in L^2(\Omega)\}.$$

The adjoint operator $B_0^* = B^*$ reads

$$\begin{aligned} B_0^*\phi &= \tau^*\phi, \\ \operatorname{Dom}(B_0^*) &= \{\phi \in L^2(\Omega) \cap W^{1,2}_{\mathrm{loc}}(\Omega \cup \partial\Omega_2) : \phi \restriction \partial\Omega_2 = 0 \text{ a.e.}, \\ &\qquad \tau^*\phi \in L^2(\Omega)\} =: \mathscr{D}^*. \end{aligned} \tag{21}$$

Proof. We start with the adjoint operator B_0^*. Let $\phi \in \mathscr{D}^*$ and $\psi \in \operatorname{Dom}(B_0)$. There exists $\chi \in C_0^\infty(\mathbb{R}^2)$ such that $\chi \restriction \operatorname{supp}\psi = 1$ and $\operatorname{supp}\chi \cap \overline{\partial\Omega_1} = \emptyset$. Then

$$\begin{aligned} \int_\Omega \overline{\phi} B_0\psi &= \int_{\operatorname{supp}\psi} \overline{\phi}\tau\psi = \int_\Omega \overline{\phi}\chi\tau\psi = \int_\Omega \overline{\tau^*(\chi\phi)}\psi = \int_{\operatorname{supp}\psi} \overline{\tau^*\phi}\psi \\ &= \int_\Omega \overline{(\tau^*\phi)}\psi, \end{aligned} \tag{22}$$

where we used that $\chi\phi \in W^{1,2}(\Omega)$ so that we can apply Gauss's theorem.

The proof of the opposite inclusion, *i.e.* $\mathrm{Dom}\,(B_0^*) \subset \mathscr{D}^*$, follows the lines of the corresponding part of the proof of Proposition 3. The compact subsets K are chosen to be in $\Omega \cup \partial\Omega_2$ and $\chi \in C_0^\infty(\mathbb{R}^2)$ so that $\chi \restriction K = 1$ and $\mathrm{supp}\,\chi \cap \overline{\partial\Omega_1} = \emptyset$. The remaining part of the proof can be completed straightforwardly according to the above mentioned proof of Proposition 3.

The inclusion of $\mathrm{Dom}\,(B) \subset \mathscr{D}$ can be justified by considering the restriction of B_0^* to $\mathscr{D}_0^* := \{\phi \in C^\infty(\overline{\Omega}) : \mathrm{supp}\,\phi \cap \overline{\partial\Omega_2} = \emptyset\}$ and proving that the adjoint of this restriction acts as τ on the domain $\mathscr{D}$. To show the latter, we can use the same strategy as in the preceding step where we described B_0^*. Consequently, $\mathrm{Dom}\,(B) = \mathrm{Dom}\,(B_0^{**}) \subset \mathscr{D}$. We show the first inclusion in (20) in two steps. The first part, *i.e.* $\mathscr{D}_0 \subset \mathrm{Dom}\,(B)$, is a consequence of the norm inequality $\|\tau\psi\|^2 + \|\psi\|^2 \leq 2\|\psi\|^2_{W^{1,2}(\Omega)}$ and the result on the closure of $\mathrm{Dom}\,(B_0)$ in $W^{1,2}$ norm, *cf.* [4, Chap.7.2] or [19, Prop.3.1.a] with the precise claim and complete proof. The second, *i.e.* $\mathscr{D}_{\mathrm{loc}} \subset \mathrm{Dom}\,(B)$, follows from $\mathscr{D}_{\mathrm{loc}} \subset \mathrm{Dom}\,(B^{**})$ which can be verified by integration by parts. □

We remark that it remains open if $\mathrm{Dom}\,(B) = \mathscr{D}$, but the derived inclusions are useful for further spectral analysis and will be sufficient for our purposes.

3. Spectral properties

We shall now focus on the spectra of the squares of the Dirac operators introduced in the previous section. The Hamiltonians with armchair boundary conditions generate "standard" Laplacians defined in $W^{2,2}$ spaces. The example with a bounded (rectangle) Ω and the combination of armchair and periodic boundary conditions is presented in Section 4.3. As can be expected, the resolvent of such an operator is compact.

The situation is different when zigzag boundary conditions are imposed. In the special case of $\partial\Omega^1 = \partial\Omega$ and $\partial\Omega^2 = \emptyset$, it has been proved in [23, Prop.3] that $A^*A = -\Delta_D$, *i.e.* the usual Dirichlet Laplacian on Ω, and 0 is an eigenvalue of AA^* with infinite multiplicity. This means, in particular, that AA^* does not have a compact resolvent which is linked with the large domain of definition – see [23] for examples and further details. In our more general situations, *i.e.* both $\partial\Omega^{1,2}$ or $\partial\Omega_{1,2}$ are non-empty, we cannot expect the domains of definition of either of the supersymmetric partners to be a standard Sobolev space as in the above mentioned particular case.

We shall show that 0 is not an eigenvalue of either TT^* or T^*T, with $T = A, B$. Nonetheless, it belongs to the essential spectrum of these operators. The typical picture is the existence of a sequence of eigenvalues converging to 0, unlike in the special case studied in [23]. This effect will be illustrated by explicitly solvable examples, namely, the annulus, *cf.* 4.2, which corresponds to the first situation with two connected components of $\partial\Omega$ and $T = A$.

In the rest of the examples, *i.e.* the annular sector and the rectangle, the zigzag boundary conditions are complemented with periodic boundary conditions – see Section 4 for details. The sequence of eigenvalues converging to zero is observed here as well and explicit calculations can be performed particularly in the simplest rectangle case. Explicit calculations may be done also for the rectangle with a combination of armchair and zigzag boundary conditions, where the same effect is observed. Examples of a similar effect in $\mathbb{R}^3$ may be found in [8, 7], where the potential perturbation is responsible for splitting the infinite dimensional kernel to the sequence of eigenvalues converging to 0. Our operators can be viewed as a perturbation in the boundary conditions of the operator in [23].

Dirac operators are known to be locally compact [24, 13] in $L^2(\mathbb{R}^3)$, *i.e.* for any compact set K, $\chi_K(H-z)^{-1}$, where χ_K is a characteristic function of K, is a compact operator. Since 0 is in the essential spectrum of the Dirac operators also for bounded Ω, its resolvent cannot be compact. Nonetheless, it still enjoys the local compactness property in Ω – see Proposition 7 for the precise meaning of this statement. As a consequence, the essential spectrum of the Dirac operator is a Zhislin one, *cf.* [12, 13] in $\mathbb{R}^n$, *i.e.* the singular sequences vanish eventually on any compact subset of Ω. As was pointed out in [23], such a behavior is clearly connected to the large domain of definition at the boundary without the Dirichlet boundary condition (or with "Cauchy-Riemann" boundary condition in the language of squares of operators).

Using a refined version of the local compactness in the first situation of "complementary" Dirichlet boundary conditions ($T = A$), we show that 0 is the only point in the essential spectrum of H^A_{zz} or AA^* and A^*A. However, this remains open in the second situation of "interchanging" Dirichlet boundary conditions ($T = B$). If zero is the only point of the essential spectrum (and it cannot be an eigenvalue), it must be the only finite accumulation point of eigenvalues. Due to the local compactness property, the sequence of corresponding eigenfunctions Ψ_n must vanish in any compact subset of Ω, more precisely $\|\chi_K\Psi_n\| \to 0$. In the physics literature such eigenstates, called edge states, have been extensively studied, see *e.g.* [10, 3, 27, 17] and are responsible for some of the unusual physical properties of graphene.

The local compactness property also enables us to use a version of Glazman's decomposition (*cf.* [7] for its application to models in $\mathbb{R}^3$), so that we can localize the essential spectrum of the Dirac operator perturbed by a bounded potential. As expected, only the values of the potential on $\partial\Omega$ will be relevant.

In what follows, we always assume that Ω is as in Propositions 3 or 4 and both $\partial\Omega^i$ and $\partial\Omega_i$ $(i = 1, 2)$ are non-empty.

Proposition 5. *Zero is not an eigenvalue of either* T^*T *or* TT^**, for* $T = A, B$*.*

Proof. We consider B^*B only, as the reasoning in the remaining cases is analogous. Assume there existed a zero eigenvalue with associated eigenfunction ψ_0. Then $t_{B^*B}[\psi_0] = \|\tau\psi_0\|^2 = 0$. Take $x_0 \in \partial\Omega_1$ and consider an open ball U_0 centred at x_0 such that $\overline{U_0} \cap \overline{\partial\Omega_2} = \emptyset$. Define $\tilde{\Omega} := \Omega \cup U_0$ and denote the zero extension of ψ_0 on $\tilde{\Omega}$ by $\tilde{\psi}_0$. Since the trace of ψ_0 is zero on $\partial\Omega_1$, the zero extension $\tilde{\psi}_0$ belongs to $W^{1,2}(U)$ for any U such that $\overline{U} \subset \tilde{\Omega}$. Moreover, for any $\phi \in C_0^\infty(\tilde{\Omega})$,

$$|\langle\phi, \tau\tilde{\psi}_0\rangle_{L^2(\tilde{\Omega})}| = |\langle\tau^*\phi, \psi_0\rangle_{L^2(\Omega)}| = |\langle\phi, \tau\psi_0\rangle_{L^2(\Omega)}| \le \|\phi\|\|\tau\psi_0\| = 0, \tag{23}$$

since $\phi \restriction \Omega \in \mathrm{Dom}\,(B^*)$. Hence $\tilde{\psi}_0$ is analytic in $\tilde{\Omega}$, *cf.* [2, Sec.9.1]. Therefore $\tilde{\psi}_0$ must vanish identically since it is zero on an open set. □

Proposition 6. *Zero is in the essential spectrum of both* T^*T *and* TT^**,* $T = A, B$*.*

Proof. We give the proof for $T = A$ only, as again the case of $T = B$ is analogous. We consider A^*A first and show below that 0 is in the spectrum. Since we have excluded the possibility of 0 being an eigenvalue, it cannot be an isolated point of the spectrum. Therefore there must be a nontrivial sequence of points in the spectrum having 0 as an accumulation point. Because of the supersymmetry, *cf.* Proposition 2, the non-zero spectrum of A^*A coincides with that of AA^* and therefore 0 is in the spectrum of AA^* as well.

To prove that 0 is in the spectrum of A^*A we use Dirichlet bracketing, supersymmetry, and a suitable singular sequence inspired by the examples below – see Proposition 12. We "cut" a rectangle $\mathcal{R} := (a_1, a_2) \times (b_1, b_2) \subset \mathbb{R}^2$ from of Ω, which intersects $\partial\Omega^2$. More precisely, we place $\mathcal{R}$ in such a way that $\Omega' := (\Omega \cap \mathcal{R})^\circ \neq \emptyset$

and the boundary of Ω' consists of three straight segments (the part of the boundary of $\mathcal{R}$, *i.e.* $\Sigma := \partial\mathcal{R} \cap \Omega$) and the part of $\partial\Omega^2$, *i.e.* Ω' is a "rectangle" with one deformed side, *e.g.* $\partial\Omega' = [a_1, a_2] \times \{b_1\} \cup \{a_1\} \times [b_1, q_1] \cup \{a_2\} \times [b_1, q_2] \cup \partial\Omega^2 \cap \overline{\mathcal{R}}$. The following procedure can be easily adapted when another part of $\partial\mathcal{R}$ is deformed.

We use a Dirichlet bracketing type argument, *i.e.* we impose additional Dirichlet boundary conditions on Σ. Define the operator $(B_D)_0$ acting as τ on functions from $\operatorname{Dom}((B_D)_0) := \{\psi \in C^\infty(\overline{\Omega'}) : \operatorname{supp}\psi \cap \overline{\Sigma} = \emptyset\}$ and denote by B_D its closure in $L^2(\Omega')$. Since $\|(B_D)_0\psi\| = \|\tau\psi\| = \|A\psi\|$ for all $\psi \in \operatorname{Dom}((B_D)_0)$, every $\varphi \in \operatorname{Dom}(B_D)$, extended by 0, belongs to $\operatorname{Dom}(A)$. The non-zero spectra of $B_D^* B_D$ and $B_D B_D^*$ coincide and $B_D B_D^*$ is associated with the quadratic form

$$
\begin{aligned}
t_{B_D B_D^*}[\phi] &:= \|\tau^*\phi\|^2, \\
\operatorname{Dom}(t_{B_D B_D^*}) &:= \big\{\phi \in L^2(\Omega') \cap W^{1,2}_{\mathrm{loc}}(\Omega' \cup (\partial\Omega^2 \cap \mathcal{R})) : \\
&\qquad \phi \restriction (\partial\Omega^2 \cap \mathcal{R}) = 0 \text{ a.e.}, \tau^*\phi \in L^2(\Omega')\big\}
\end{aligned}
\tag{24}
$$

by Propositions 2 and 4. We define a sequence $\{\phi_n\} \subset \operatorname{Dom}(t_{B_D B_D^*}) = \operatorname{Dom}(B_D^*)$

$$
\phi_n(x_1, x_2) := \begin{cases} e^{-inx_1} \sinh n(q - x_2), & x_2 < q, \\ 0, & x_2 \geq q, \end{cases}
\tag{25}
$$

where $q > 0$ is such that $[a_1, a_2] \times [b_1, q] \subset \Omega'$ and we get that $\|\tau^*\phi_n\|/\|\phi_n\| \to 0$. Therefore zero is in the spectrum of $B_D B_D^*$ and, since by Proposition 5 it cannot be an eigenvalue, it must be an accumulation point of the spectrum. By supersymmetry, 0 is an accumulation point of the spectrum of $B_D^* B_D$ as well, *i.e.* $0 \in \sigma_{\mathrm{ess}}(B_D^* B_D)$. The latter implies the existence of the sequence of functions $\psi_n \in \operatorname{Dom}(B_D)$ such that $\|\psi_n\| = 1$ and $\|B_D\psi_n\| = \|\tau\psi_n\| = \|A\psi_n\| \to 0$, thus 0 is in the spectrum of A^*A. $\square$

Further spectral results are mainly based on local compactness.

Proposition 7. *Let* $\varphi_i, \xi_i \in C_0^\infty(\mathbb{R}^2)$ $(i = 1, 2)$ *be such that* $\operatorname{supp}\xi_i \subset \Omega \cup \partial\Omega_i$ $(i = 1, 2)$*,* $\operatorname{supp}\varphi_1 \cap \partial\Omega^2 = \emptyset$ *and* $\operatorname{supp}\varphi_2 \cap \partial\Omega^1 = \emptyset$*. Then*

$$
\begin{pmatrix} \varphi_1 & 0 \\ 0 & \varphi_2 \end{pmatrix} \begin{pmatrix} -z & A^* \\ A & -z \end{pmatrix}^{-1}, \qquad \begin{pmatrix} \xi_1 & 0 \\ 0 & \xi_2 \end{pmatrix} \begin{pmatrix} -z & B^* \\ B & -z \end{pmatrix}^{-1}
\tag{26}
$$

are compact operators in $L^2(\Omega, \mathbb{C}^2)$ *for any* $z \in \mathbb{C} \setminus \mathbb{R}$*.*

Proof. We prove the compactness of the first operator only, the second proof being analogous. Let $\Psi \in L^2(\Omega, \mathbb{C}^2)$ and denote $\Phi := (H^A_{\mathrm{zz}} - z)^{-1}\Psi$. Since Φ_1 and Φ_2 belong to $\operatorname{Dom}(A)$ and $\operatorname{Dom}(A^*)$, respectively, $\varphi_i\Phi_i \in W^{1,2}_0(\Omega)$. We show that the operator in (26) is bounded when considered as a mapping $L^2(\Omega, \mathbb{C}^2) \to W^{1,2}(\Omega, \mathbb{C}^2)$. To this end we estimate the $W^{1,2}$ norm of $\varphi_i\Phi_i$. The basic step is to notice that $\|\varphi_i\Phi_i\|^2_{W^{1,2}(\Omega)} = \|\tau(\varphi_i\Phi_i)\|^2 + \|\varphi_i\Phi_i\|^2 = \|\tau^*(\varphi_i\Phi_i)\|^2 + \|\varphi_i\Phi_i\|^2$. Then

$$
\begin{aligned}
\sum_{i=1}^{2} \|\varphi_i\Phi_i\|^2_{W^{1,2}} &= \|\tau(\varphi_1\Phi_1)\|^2 + \|\varphi_1\Phi_1\|^2 + \|\tau^*(\varphi_2\Phi_2)\|^2 + \|\varphi_2\Phi_2\|^2 \\
&\leq 2\big(\|\tau\varphi_1\|^2_\infty\|\Phi_1\|^2 + \|\varphi_1\|^2_\infty\|\tau\Phi_1\|^2 + \|\tau^*\varphi_2\|^2_\infty\|\Phi_2\|^2 \\
&\qquad + \|\varphi_2\|^2_\infty\|\tau^*\Phi_2\|^2\big) + \|\varphi_1\Phi_1\|^2 + \|\varphi_2\Phi_2\|^2 \\
&\leq C_1(\|(H^A_{\mathrm{zz}} - z)\Phi + z\Phi\|^2 + \|\Psi\|^2) \leq C_2\|\Psi\|^2,
\end{aligned}
\tag{27}
$$

where C_2 is independent of Ψ. Mapping $\operatorname{diag}(\varphi_1, \varphi_2)\Phi$ to $L^2(\Omega, \mathbb{C}^2)$ gives the claim by the compact embedding of the Sobolev space in the L^2 space. $\square$

Proposition 8. *Let $\lambda \in \sigma_{\rm ess}(H^T_{\rm zz})$, with $T = A, B$, let φ_i, ξ_i $(i = 1, 2)$ be as in Proposition 7 and let $K^i, K_i \subset \mathbb{R}^2$ be compact sets such that $K^i \subset \Omega \cup \partial\Omega^i$ and $K_i \subset \Omega \cup \partial\Omega_i$ $(i = 1, 2)$. Let also $\{\Psi^T_n\} \subset \mathrm{Dom}\,(T)$ be a singular sequence for λ, i.e. $\|\Psi^T_n\| = 1$, $\Psi^T_n \xrightarrow{\rm w} 0$, $\|(H^T_{\rm zz} - \lambda)\Psi^T_n\| \to 0$. Then $\varphi_i(\Psi^A_n)_i \to 0$ $(i = 1, 2)$ and $\xi_i(\Psi^B_n)_i \to 0$ $(i = 1, 2)$. Moreover, for $\lambda = 0$, the singular sequence $\{\Psi^T_n\}$ can be selected such that $(\Psi^A_n)_i \restriction K^i = 0$, $(\Psi^B_n)_i \restriction K_i = 0$ in addition.*

Proof. We give the proof for $T = A$ and simplify the notation $\Psi^T_n \equiv \Psi_n$, $H^T_{\rm zz} \equiv H_{\rm zz}$. We denote $\tilde{\varphi}_i := (1 - \varphi_i)$. Using the identity (for $z \in \mathbb{C} \setminus \mathbb{R}$)

$$\begin{aligned} \begin{pmatrix} \varphi_1 & 0 \\ 0 & \varphi_2 \end{pmatrix} \Psi_n = \begin{pmatrix} \varphi_1 & 0 \\ 0 & \varphi_2 \end{pmatrix} (H_{\rm zz} - z)^{-1}(H_{\rm zz} - \lambda)\Psi_n + \\ (\lambda - z) \begin{pmatrix} \varphi_1 & 0 \\ 0 & \varphi_2 \end{pmatrix} (H_{\rm zz} - z)^{-1}\Psi_n \end{aligned} \tag{28}$$

we get by the local compactness that $\varphi_i(\Psi_n)_i \to 0$.

For $\lambda = 0$, we fix φ_i such that $\operatorname{supp}\varphi_i \cap \overline{\Omega} \subset \Omega \cup \partial\Omega^i$ and $\varphi_i = 1$ on an ε-neighborhood of K^i (for ε small enough); it follows that $\tilde{\varphi}_i \restriction K^i = 0$. We define $\Phi_n := \|\mathrm{diag}(\tilde{\varphi}_1, \tilde{\varphi}_2)\Psi_n\|^{-1}\mathrm{diag}(\tilde{\varphi}_1, \tilde{\varphi}_2)\Phi_n$, hence $(\Phi_n)_i \restriction K^i = 0$ and $\Phi_n \xrightarrow{\rm w} 0$. Note that Φ_n is correctly defined since, for $n > n_0$,

$$\|\mathrm{diag}(\tilde{\varphi}_1, \tilde{\varphi}_2)\Psi_n\| \geq 1 - \|\mathrm{diag}(\varphi_1, \varphi_2)\Psi_n\| \geq c > 0. \tag{29}$$

Finally,

$$\|H_{\rm zz}\Phi_n\| \leq \frac{1}{c}\left(\left\| \begin{pmatrix} (\Psi_n)_2\tau^*\varphi_2 \\ (\Psi_n)_1\tau\varphi_1 \end{pmatrix} \right\| + \|\mathrm{diag}(\tilde{\varphi}_2, \tilde{\varphi}_1)H_{\rm zz}\Psi_n\|\right), \tag{30}$$

hence $\{\Phi_n\}$ is a singular sequence for $\lambda = 0$ since Ψ_n is a singular sequence for $\lambda = 0$, $\varphi_i(\psi_n)_i \to 0$ and $(\Psi_n)_i\tau^*\varphi_i$ (the latter follows from the first part of the claim and $\operatorname{supp}\tau\varphi_1 \subset \operatorname{supp}\varphi_1$, $\operatorname{supp}\tau^*\varphi_2 \subset \operatorname{supp}\varphi_2$). □

Proposition 9. $\sigma_{\rm ess}(H^A_{\rm zz}) = \sigma_{\rm ess}(A^*A) = \sigma_{\rm ess}(AA^*) = \{0\}$ *and* 0 *is not an eigenvalue.*

Proof. Denote $H^A_{\rm zz} \equiv H_{\rm zz}$. Let us assume that $\lambda \in \sigma_{\rm ess}(H_{\rm zz})$ and take a corresponding singular sequence $\{\Psi_n\}$. Direct manipulations yield

$$\begin{aligned} \|(H_{\rm zz} - \lambda)\Psi_n\|^2 &= \|\tau(\Psi_n)_1 - \lambda(\Psi_n)_2\|^2 + \|\tau^*(\Psi_n)_2 - \lambda(\Psi_n)_1\|^2 \\ &= \|\tau(\Psi_n)_1\|^2 + \|\tau^*(\Psi_n)_2\|^2 + |\lambda|^2 \\ &\quad - 4\lambda\mathrm{Re}\,\langle\tau^*(\Psi_n)_2, (\Psi_n)_1\rangle. \end{aligned} \tag{31}$$

With the help of Proposition 8, we show below that $\langle\tau^*(\Psi_n)_2, (\Psi_n)_1\rangle \to 0$. However, since $\|(H_{\rm zz} - \lambda)\Psi_n\| \to 0$, (31) gives that λ must be 0.

It remains to prove that $\langle\tau^*(\Psi_n)_2, (\Psi_n)_1\rangle \to 0$. Take φ_1 as in Proposition 7 and denote $\tilde{\varphi_1} := (1 - \varphi_1)$. Using integration by parts, we obtain

$$\begin{aligned} |\langle\tau^*(\Psi_n)_2, (\Psi_n)_1\rangle| \leq |\langle\tau^*(\Psi_n)_2, \varphi_1(\Psi_n)_1\rangle| + |\langle(\Psi_n)_2, (\Psi_n)_1\tau\varphi_1\rangle| \\ + |\langle\tilde{\varphi}_1(\Psi_n)_2, \tau(\Psi_n)_1\rangle|. \end{aligned} \tag{32}$$

Since $\operatorname{supp}\tau\varphi_1 \subset \operatorname{supp}\varphi_1$ and $\operatorname{supp}\tilde{\varphi}_1 \cap \partial\Omega^1 = \emptyset$, all terms on the right hand side tend to 0 by Proposition 8 and the fact that $\|\tau(\Psi_n)_1\| + \|\tau^*(\Psi_n)_2\| \leq M < \infty$. The later follows from the first equality in (31), $(H_{\rm zz} - \lambda)\Psi_n \to 0$ and $\|\Psi_n\| = 1$.

□

Finally, we examine the effect of a perturbation by a bounded real potential V on the essential spectrum.

Proposition 10. *Let $V \in L^\infty(\Omega)$ be a real potential. Let $U_\delta := \{x \in \Omega : \operatorname{dist}(x, \partial\Omega) < \delta\}$ and let denote $m_\delta := \operatorname{ess\,inf}_{U_\delta} V$, $M_\delta := \operatorname{ess\,sup}_{U_\delta} V$. Then $\sigma_{\mathrm{ess}}(H_{zz}^A + V) \subset \cap_{\delta>0}[m_\delta, M_\delta]$.*

Proof. We begin by showing that the localization of the essential spectrum does not depend on the potential inside Ω. More precisely $\sigma_{\mathrm{ess}}(H_{\mathrm{zz}} + V) = \sigma_{\mathrm{ess}}(H_{\mathrm{zz}} + (1 - \chi_K)V)$, where χ_K is the characteristic function of a compact set $K \subset \Omega$ and $H_{\mathrm{zz}} \equiv H_{\mathrm{zz}}^A$. From Proposition 7, it follows that $\chi_K(H_{\mathrm{zz}} - z)^{-1}$ is compact. Hence $\chi_K(H_{\mathrm{zz}} + V - z)^{-1} = \chi_K(H_{\mathrm{zz}} - z)^{-1} - \chi_K(H_{\mathrm{zz}} - z)^{-1}V(H_{\mathrm{zz}} + V - z)^{-1}$ is compact, *i.e.* $H_{\mathrm{zz}} + V$ remains locally compact. As a consequence, $\chi_K V$ is a relatively compact perturbation of $H_{\mathrm{zz}} + V$.

For positive δ we define $K \equiv K_\delta := \Omega \setminus U_\delta$. Then there exists a singular sequence $\{\Psi_n\}$ for H_{zz} and $\lambda = 0$ such that $\Psi_n \upharpoonright K = 0$. Similarly as in [7, Thm.8], we show by [11, Thm.10] that for every $\varepsilon > 0$, the interval $(m_\delta - \varepsilon, M_\delta + \varepsilon)$ contains an infinite set of points of the spectrum of $H_{\mathrm{zz}} + V$. For all $n > n(\varepsilon)$,

$$\begin{aligned} &\|(H_{\mathrm{zz}} + V - \frac{1}{2}(M_\delta + m_\delta))\Psi_n\| \leq \|H_{\mathrm{zz}}\Psi_n\| + \|(V - \frac{1}{2}(M_\delta + m_\delta))\Psi_n\| \\ &< (\varepsilon + \frac{1}{2}(M_\delta - m_\delta))\|\Psi_n\| \end{aligned} \tag{33}$$

Finally, let $\lambda > M_\delta$. We prove that λ is not in $\sigma_{\mathrm{ess}}(H + V_\delta)$, where $V_\delta(x) := m_\delta\chi_K + (1 - \chi_K)V$, *i.e.* we change the potential on K. The argument is based on [11, Thm.6]. Since $\lambda - m_\delta > M_\delta - m_\delta \geq 0$, there exists, *cf.* [11, Thm.6], a positive number ε and a subspace F with finite deficiency such that for all $\varphi \in F \cap \mathrm{Dom}\,(H_{\mathrm{zz}})$

$$\|(H_{\mathrm{zz}} - (\lambda - m_\delta)\varphi\| > (M_\delta - m_\delta + \varepsilon)\|\varphi\|. \tag{34}$$

It follows that for all $\varphi \in F \cap \mathrm{Dom}\,(H_{\mathrm{zz}})$ we have

$$\begin{aligned} &\|(H_{\mathrm{zz}} + V_\delta - \lambda)\varphi\| \geq \|(H_{\mathrm{zz}} - (\lambda - m_\delta))\varphi\| - \|(V_\delta - m_\delta)\varphi\| \\ &> (M_\delta - m_\delta + \varepsilon)\|\varphi\| - (M_\delta - m_\delta)\|\varphi\| = \varepsilon\|\varphi\|. \end{aligned} \tag{35}$$

Hence $\lambda \notin \sigma_{\mathrm{ess}}(H_{\mathrm{zz}} + V_\delta) = \sigma_{\mathrm{ess}}(H_{\mathrm{zz}} + V)$. An analogous argument can be given for $\lambda < m_\delta$. □

If V is continuous on $\overline{\Omega}$, the essential spectrum of $H_{\mathrm{zz}} + V$ lies between the minimum and maximum of V on $\partial\Omega$.

A weaker result can be obtained also for $H_{\mathrm{zz}}^B + V$, namely $\sigma_{\mathrm{ess}}(H_{\mathrm{zz}}^B + V) \cap (\cap_{\delta>0}[m_\delta, M_\delta]) \neq \emptyset$. The difficulty in describing the entire essential spectrum lies in the fact that we do not know if zero is the only point of the essential spectrum of H_{zz}^B.

Remark 1. Using the existence of singular sequences from Proposition 6 with $T = B$, we can in fact improve the result on the localization of the essential spectrum of $H_{\mathrm{zz}}^A + V$. Let $x_0 \in \partial\Omega$, $U_\delta(x_0) := \{x \in \Omega : \operatorname{dist}(x_0, x) < \delta\}$, and $m_\delta(x_0) := \operatorname{ess\,inf}_{U_\delta(x_0)} V$, $M_\delta(x_0) := \operatorname{ess\,sup}_{U_\delta(x_0)} V$. Then $\sigma_{\mathrm{ess}}(H_{\mathrm{zz}}^A + V) \cap (\cap_{\delta>0}[m_\delta(x_0), M_\delta(x_0)]) \neq \emptyset$.

To see this, the Dirichlet bracketing argument is used as in Proposition 6. Let us assume that $x_0 \in \partial\Omega^2$ and consider a sequence $\{\psi_n\} \subset \mathrm{Dom}\,(A)$ localizing at $\partial\Omega^2$ and being zero outside of $\overline{U_\delta(x_0)}$, such that $\|\tau\psi_n\| \to 0$. Inserting this sequence in [11, Thm.10], *i.e.* the estimate of type (33), yields the claim.

4. Examples

We shall now consider several examples based on rectangles, sectors and annulus, to illustrate the operators studied in the previous sections. In addition to armchair and zigzag boundary conditions, in some instances we shall complement these with periodic boundary conditions. In view of the Dirac equation in a curved space and its connection to graphene, see *e.g.* [5, 25, 15], the examples of rectangles with periodic boundary conditions can be viewed as models on a cylinder or cone (if the frame is chosen as in [5, Eq.(A12)]) in $\mathbb{R}^3$. Information on the spectra of such operators also provides insight on how to deal with waveguides, *i.e.* Ω is an infinite strip, which we consider in Section 5 below.

4.1. **Rectangle with zigzag and periodic boundary conditions.** Let Ω be the rectangle $\Omega := (-a,a) \times (-b,b)$ and write

$$\begin{array}{lllllll} \partial\Omega_1 & := & (-a,a)\times\{-b\} & \quad & \partial\Omega_2 & := & (-a,a)\times\{b\} \\ \partial\Omega_3 & := & \{-a\}\times(-b,b) & \quad & \partial\Omega_4 & := & \{a\}\times(-b,b) \end{array}. \tag{36}$$

We realize the differential expression H_1 from (8) as a self-adjoint operator H_{zp} in $L^2(\Omega)$.

Proposition 11. *Let A be the operator defined by $A\psi := \tau\psi$ on*

$$\begin{aligned} \mathrm{Dom}\,(A) := \big\{&\psi \in L^2(\Omega) : \forall\varepsilon > 0, \psi \in W^{1,2}((-a,a)\times(-b,b-\varepsilon)), \\ &\psi \restriction \partial\Omega_1 = 0,\ \psi \restriction \partial\Omega_3 = \psi \restriction \partial\Omega_4 \text{ a.e.}, \tau\psi \in L^2(\Omega)\big\}. \end{aligned} \tag{37}$$

Then A is closed and A^* is given by

$$\begin{aligned} &A^*\phi = \tau^*\phi, \\ &\mathrm{Dom}\,(A^*) = \big\{\phi \in L^2(\Omega) : \forall\varepsilon > 0, \psi \in W^{1,2}((-a,a)\times(-b+\varepsilon,b)), \\ &\qquad \phi \restriction \partial\Omega_2 = 0,\ \phi \restriction \partial\Omega_3 = \phi \restriction \partial\Omega_4 \text{ a.e.}, \tau^*\phi \in L^2(\Omega)\big\}. \end{aligned} \tag{38}$$

Proof. We denote by $\mathscr{D}^*$ the set on the right hand side of (38) and take $\phi \in \mathscr{D}^*$. We show that $\phi \in \mathrm{Dom}\,(A^*)$. Any $\psi \in \mathrm{Dom}\,(A)$ restricted to $\Omega_- := (-a,a)\times(-b,0)$ is in $W^{1,2}(\Omega_-)$ and satisfies Dirichlet and periodic boundary conditions respectively on $\partial\Omega_1$ and the part of $\partial\Omega_i$ $(i = 3,4)$, namely on $\{-a\}\times(-b,0)$ and $\{a\}\times(-b,0)$. Similarly, ϕ restricted to $\Omega_+ := (-a,a)\times(0,b)$ is in $W^{1,2}(\Omega_+)$ and satisfies Dirichlet and periodic boundary conditions on $\partial\Omega_2$ and the part of $\partial\Omega_i$ $(i = 3,4)$.

Both ψ and ϕ can be approximated on Ω_-, Ω_+, respectively, in the $W^{1,2}$ norm by smooth functions ψ_n and ϕ_n, whose supports do not intersect $\overline{\partial\Omega_1}$, $\overline{\partial\Omega_2}$, respectively, and satisfying also the periodic boundary conditions in the corresponding part of the boundary. Then

$$\int_\Omega \overline{\phi}\tau\psi = \lim_{n\to\infty}\int_{\Omega_-} \overline{\phi}\tau\psi_n + \lim_{n\to\infty}\int_{\Omega_+} \overline{\phi_n}\tau\psi = \int_\Omega \overline{\tau^*\phi}\psi, \tag{39}$$

since the boundary terms vanish on $\partial\Omega_i$ $(i = 1,2)$ and cancel on $\partial\Omega_i$ $(i = 3,4)$ and $(-a,a)\times\{0\}$.

The operator A is an extension of A_0 acting as τ on

$$\begin{aligned} \mathrm{Dom}\,(A_0) \quad := \quad &\{\psi \in C^\infty(\Omega) : \exists\psi_0 \in C_0^\infty(\mathbb{R}^2), \psi = \psi_0 \restriction \Omega, \\ &\mathrm{supp}\,\psi_0 \cap (\overline{\partial\Omega_1} \cup \overline{\partial\Omega_3} \cup \overline{\partial\Omega_4}) = \emptyset\}. \end{aligned}$$

By Proposition 4, the domain of the adjoint of A_0 is

$$\mathrm{Dom}\,(A_0^*) \quad = \quad \{\phi \in L^2(\Omega) \cap W^{1,2}_{\mathrm{loc}}(\Omega \cup \partial\Omega_2) : \phi \restriction \partial\Omega_2 = 0 \text{ a.e.}\tau^*\phi \in L^2(\Omega)\},$$

and clearly $\mathrm{Dom}\,(A^*) \subset \mathrm{Dom}\,(A_0^*)$. For non-negative values of t we introduce the (bounded) shift operators T_t defined by

$$(T_t\psi)(x_1,x_2) := \begin{cases} \psi(x_1+t,x_2), & \text{if } x_1+t \le a, \\ \psi(x_1+t-2a,x_2), & \text{if } x_1+t > a. \end{cases} \tag{40}$$

If ψ is $2a$-periodic in x_1, T_t acts as the usual shift operator. It is easy to verify that $T_t^* = T_t^{-1} = T_{-t}$, where

$$(T_{-t}\psi)(x_1,x_2) := \begin{cases} \psi(x_1-t,x_2), & \text{if } x_1-t \geq -a, \\ \psi(x_1-t+2a,x_2), & \text{if } x_1-t < -a. \end{cases} \tag{41}$$

Since $A = T_{-t}AT_t$ and T_t is bounded with bounded inverse, the same equality is valid for the adjoints, *i.e.* $A^* = T_{-t}A^*T_t$. This equality particularly means that if $\phi \in \operatorname{Dom}(A^*)$, then $T_t\phi \in \operatorname{Dom}(A^*)$ which implies (with regard to the domain inclusion) that $\operatorname{Dom}(A^*) \subset \{\phi \in L^2(\Omega) : \forall\varepsilon > 0, \psi \in W^{1,2}((-a,a)\times(-b+\varepsilon,b)), \phi \restriction \partial\Omega_2 = 0, \tau^*\phi \in L^2(\Omega)\}$. Taking suitable $\psi \in \operatorname{Dom}(A)$, namely those whose support does not intersect $\overline{\partial\Omega_1}$, and using integration by parts, we see that functions from $\operatorname{Dom}(A^*)$ also satisfy periodic boundary conditions.

Repeating the described procedure yields $A = A^{**}$. □

Having proven that H_{zp} is self–adjoint, we shall now study its spectrum. In fact, we study the spectrum of H_{zp}^2 from which the spectrum of H_{zp} can be deduced. Formal calculations directly for H_{zp} may be found in [3, 27]. Because of the symmetry, the operators on the diagonal of H_{zp}^2 have the same spectrum.

Proposition 12. *Let A and A^* be the operators from Proposition 11. Then the essential spectrum of A^*A consists only of zero and its eigenvalues may be written as $\lambda_{m,n} = \sigma_m^2 + \omega_{m,n}^2$, where $\sigma_m = (m\pi)/a$ with $m \in \mathbb{Z}$ and $\omega_{m,n}^2$, $m \in \mathbb{Z}$, $n \in \mathbb{N}$, are the eigenvalues of the one-dimensional Dirichlet-Robin problems (indexed by n in increasing order)*

$$\begin{cases} -\xi'' = \omega_{m,n}^2\xi & \text{in } (-b,b), \\ \xi = 0 & \text{at } -b, \\ \xi' - \sigma_m\xi = 0, & \text{at } b, \end{cases} \tag{42}$$

i.e. $\omega_{m,n}^2$ *can be obtained from the solutions of the equation*

$$\sigma_m \sin(2\omega b) = \omega\cos(2\omega b). \tag{43}$$

Eigenvalues $\lambda_{m,1} \to 0$ as $m \to +\infty$, more precisely

$$\lambda_{m,1} = 4\sigma_m^2 e^{-4\sigma_m b} + \mathcal{O}(\sigma_m^4 e^{-8\sigma_m b}). \tag{44}$$

Remark 2. If $m > m_0 := a/(2\pi b)$, then (43) yields one purely imaginary root $\omega_{m,1} = \mathrm{i}\tilde{\omega}_{m,1}$ and infinitely many positive roots $\omega_{m,n}$ satisfying:

$$\begin{aligned} n > 1 : \qquad & \frac{(n-1)\pi}{2b} \leq \omega_{m,n} \leq \frac{(2n-1)\pi}{4b}, \\ \sigma_m > \frac{2}{b},\ n = 1 : \quad & \frac{\sigma_m}{2}\left(1 + \sqrt{1 - \frac{2}{b\sigma_m}}\right) \leq \tilde{\omega}_{m,1} \leq \sigma_m. \end{aligned} \tag{45}$$

Hence

$$\lim_{m\to+\infty} \sigma_m^2 + \omega_{m,1}^2 = \lim_{m\to+\infty} \sigma_m^2 - \tilde{\omega}_{m,1}^2 = 0. \tag{46}$$

If $m < m_0 := a/(2\pi b)$, then (43) yields infinitely many positive roots $\omega_{m,n}$ satisfying:

$$\begin{aligned} 0 < m < m_0 : \quad & \frac{(n-1)\pi}{2b} \leq \omega_{m,n} \leq \frac{(2n-1)\pi}{4b}, \\ m \leq 0 : \quad & \frac{(2n-1)\pi}{4b} \leq \omega_{m,n} \leq \frac{n\pi}{2b}. \end{aligned} \tag{47}$$

The eigenfunctions

$$\Psi_{m,n}(x_1,x_2) := A_{m,n}e^{-\mathrm{i}\sigma_m x_1}\sin(\omega_{n,m}(x_2+b)), \tag{48}$$

associated to the eigenvalues $\lambda_{m,n}$ and where $A_{m,n}$ are normalization constants, form an orthonormal basis of $L^2(\Omega)$.

Proof. We search for eigenfunctions by separation of variables writing $\Psi(x_1, x_2) = \kappa(x_1)\xi(x_2)$. Assuming that Ψ is regular enough, we want to solve the following problem

$$\begin{aligned} -\Delta\Psi &= \lambda\Psi, \\ \Psi \restriction \partial\Omega_1 &= 0, \\ (\mathrm{i}\partial_1 - \partial_2)\Psi \restriction \partial\Omega_2 &= 0, \\ \Psi \restriction \partial\Omega_3 &= \Psi \restriction \partial\Omega_4, \\ \partial_1\Psi \restriction \partial\Omega_3 &= \partial_1\Psi \restriction \partial\Omega_4, \end{aligned} \tag{49}$$

and inserting Ψ as above into (49) we are led to the following equations for κ and ξ

$$\begin{aligned} -\kappa''(x_1)\xi(x_2) - \kappa(x_1)\xi''(x_2) &= \lambda\kappa(x_1)\xi(x_2), \\ \xi(-b) &= 0, \\ \mathrm{i}\kappa'(x_1)\xi(b) - \kappa(x_1)\xi'(b) &= 0, \\ \kappa(-a) = \kappa(a), \quad \kappa'(-a) &= \kappa'(a). \end{aligned} \tag{50}$$

It follows that

$$\begin{aligned} \kappa(x_1) &= C_1 e^{-\mathrm{i}\sigma x_1}, \\ \sigma &= \frac{\xi'(b)}{\xi(b)}, \\ \xi(x_2) &= C_2 \sin(\omega(x+b)), \\ \lambda &= \sigma^2 + \omega^2. \end{aligned} \tag{51}$$

The periodic boundary conditions for κ restrict the values of σ to $\sigma_m = m\pi/a$, $m \in \mathbb{Z}$. Regarding the relation between σ and the boundary values of ξ and ξ' at b, *cf.* (51), the function ξ must satisfy the Dirichlet-Robin problem (42) and $\omega_{m,n}$ the eigenvalue equation (43) in the claim.

For every $m > m_0$, we rewrite equation (43) for $\omega = \mathrm{i}\tilde{\omega}$ as

$$\tanh(2\tilde{\omega}b) = \frac{\tilde{\omega}}{\sigma_m} \tag{52}$$

and a simple analysis shows that it has one (and only one) positive root $\tilde{\omega}_{m,1}$. Furthermore, the sequence $\{\tilde{\omega}_{m,1}\}_{m_0}^{+\infty}$ is increasing and $\tilde{\omega}_{m,1} \to +\infty$ as $m \to +\infty$. If we write σ_m from (52) as a function of b and $\tilde{\omega}$ and insert it into the equation $\lambda_{m,1} = \sigma_m^2 - \tilde{\omega}_{m,1}^2$ we conclude that $\lambda_{m,1} \to 0$ as $m \to +\infty$. This also proves that 0 is in the essential spectrum of A^*A. The enclosures for $\omega_{m,n}$ in the claim follow from elementary estimates for the roots of (43) and (52).

To obtain the asymptotics of $\lambda_{m,1}$, we have to study the behaviour of the positive root of (52) for large m. Writing $\tilde{\omega}_{m,1} = \sigma_m - \varepsilon$ we obtain

$$\varepsilon(e^{-4\sigma_m b} + e^{-4\varepsilon b}) = 2\sigma_m e^{-4\sigma_m b} \tag{53}$$

and after expanding $e^{-4\varepsilon b}$ into a Taylor series around zero this yields the following equation for ε

$$\varepsilon(1 - e^{-4\sigma_m b}) - 2\sigma_m e^{-4\sigma_m b} = R(\varepsilon). \tag{54}$$

Here $R(\varepsilon) = \mathcal{O}(\varepsilon^2)$ and it is a continuous function of ε. Using *e.g.* the intermediate value theorem, it is possible to show that the solution of (54) will be of the form $\varepsilon_m = 2\sigma_m e^{-4\sigma_m b} + \mathcal{O}(\sigma_m^2 e^{-8\sigma_m b})$. Returning back to $\tilde{\omega}_{m,1}$, we obtain the expression for $\lambda_{m,1}$ in the claim.

$\mathscr{B} := \{\Psi_{m,n}\}_{m\in\mathbb{Z},n\in\mathbb{N}}$ is an orthonormal basis of $L^2(\Omega)$ since (properly normalized) $\{\kappa_m\}_{m\in\mathbb{Z}}$ and $\{\xi_{m,n}\}_{n\in\mathbb{N}}$ (for every m) are orthonormal bases of $L^2((-a,a))$ and $L^2((-b,b))$ respectively.

Since $\mathscr{B}$ is an orthonormal basis, no points other than $\lambda_{m,n}$ can be in the point spectrum and also

$$\|(A^*A-\lambda)f\|^2 = \sum_{m\in\mathbb{Z},n\in\mathbb{N}} |\langle\Psi_{m,n},f\rangle|^2|\lambda_{n,m}-\lambda|^2 \geq \inf_{m,n}|\lambda_{n,m}-\lambda|^2\|f\|^2. \tag{55}$$

Therefore only accumulation points of $\{\lambda_{m,n}\}$ can be in the essential spectrum. Using the enclosures of $\omega_{m,n}$ and values of σ_m we conclude that 0 is the only accumulation point of $\{\lambda_{m,n}\}$ and thus there are no other points in the spectrum of A^*A. $\square$

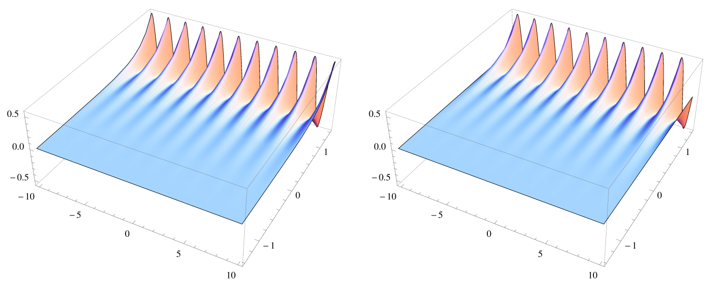

FIGURE 3. Real and imaginary part of $\Psi_{10,1}$ from Example 4.1 for $a=10$, $b=1.4$.

The spectrum of the original Dirac operator H_{zp} may now be obtained simply by taking plus and minus square root of the points in $\sigma(H_{\mathrm{zp}}^2)$.

Lemma 13. *The essential and point spectra of H_{zp} are given by $\sigma_{\mathrm{ess}}(H_{\mathrm{zp}})=\{0\}$ and $\sigma_{\mathrm{p}}(H_{\mathrm{zp}})=\{\pm\sqrt{\lambda_{m,n}}\}_{m\in\mathbb{Z},\,n\in\mathbb{N}}$, respectively. The eigenfunctions corresponding to $\pm\sqrt{\lambda_{m,n}}$ are, respectively, of the form*

$$\Phi^{\pm}_{m,n}(x_1,x_2) = A^{\pm}_{m,n}e^{-\mathrm{i}\sigma_m x_1}\begin{pmatrix}\mp\sin(\omega_{m,n}(x_2+b))\\ \sin(\omega_{m,n}(x_2-b))\end{pmatrix} \tag{56}$$

Proof. It suffices to verify by a straightforward calculation that $\Phi^{\pm}_{m,n}$ are indeed eigenfunctions associated to $\pm\sqrt{\lambda}$. $\square$

Although H_{zp}^2 acts locally as a Laplacian, its resolvent is not compact and 0 is in the essential spectrum. The latter is, in fact, a consequence of Proposition 6. In more detail, we can consider a small rectangle placed at $\partial\Omega^2$, impose additional Dirichlet boundary conditions on the other three parts of its boundary and use the sequence ψ_n from the proof of Proposition 6 to show that $\|\tau\psi_n\|\to 0$. Nonetheless, in this example we can find the singular sequence explicitly, namely $\Psi_{m,1}$. Figure 3 illustrates characteristic features of these eigenfunctions, as m increases, the eigenfunctions localize more and more near the boundary where the "Cauchy-Riemann" boundary condition is imposed.

4.2. **Annular sector with zigzag and periodic boundary conditions.** As another example, we consider $\Omega := \{(x_1,x_2) : x_1 = r\cos\varphi, x_2 = r\sin\varphi, r\in(r_1,r_2), \varphi\in(0,\alpha)\}$, *i.e.* the sector of an annulus or the entire annulus, and we impose the combination of the zigzag and periodic boundary conditions. With regard to the symmetries of Ω we further work in polar coordinates (r, φ) and denote $\tilde{\Omega}_{\mathrm{p}} := (r_1, r_2) \times (0, \alpha)$. We can start with a symmetric operator $\dot{H}^{\mathrm{a}}_{\mathrm{zp}}$

$$\begin{aligned} &\dot{H}^{\mathrm{a}}_{\mathrm{zp}}\Psi := H_1\Psi, \\ &\mathrm{Dom}\,(\dot{H}^{\mathrm{a}}_{\mathrm{zp}}) := \big\{\Psi \in C^1(\overline{\Omega}_{\mathrm{p}}) : \forall\alpha, \Psi_1(r_1, \alpha) = 0, \Psi_2(r_2, \alpha) = 0, \\ &\qquad\qquad \forall r, \Psi_{1,2}(r, 0) = \Psi_{1,2}(r, \alpha)\big\}. \end{aligned} \tag{57}$$

and describe the domain of the closure $H^{\mathrm{a}}_{\mathrm{zp}}$ of $\dot{H}^{\mathrm{a}}_{\mathrm{zp}}$ using the ideas from the previous example. If $\alpha = 2\pi$, *i.e.* Ω is entire annulus, the domain is described in Proposition 3. However, we omit further details and only calculate the eigenvalues and eigenfunctions of $(H^{\mathrm{a}}_{\mathrm{zp}})^2$.

We find the same effect as in the previous example, namely the existence of a sequence of eigenvalues converging to zero with eigenfunctions localizing to the boundary. In the case of $r_1 = 0$, *i.e.* the annulus sector becomes a usual sector, the situation is different ($\partial\Omega^1 = \emptyset$ in the notation of previous section) and we return to the example in [23] where zero is the eigenvalue of infinite multiplicity instead of having the sequence tending to zero.

Proposition 14. *Spectrum of* $(H^{\mathrm{a}}_{\mathrm{zp}})^2$ *consists of eigenvalues* $\lambda_{m,n}$, $m \in \mathbb{Z}$, $n \in \mathbb{N}$, *that are the solutions of transcendental equation* (63) *where* $\lambda = k^2$. *The associated eigenfunctions* $\psi_{m,n}(r, \varphi) = \rho_{m,n}(r)\kappa_m(\varphi)$, cf. (60)–(62), *form orthonormal basis of* $L^2(\Omega_{\mathrm{p}})$. *Eigenvalues* $\lambda_{m,1} \to 0$ *as* $m \to -\infty$ *and* $\sigma_{\mathrm{ess}}((H^{\mathrm{a}}_{\mathrm{zp}})^2) = \{0\}$.

Proof. The differential expressions τ, τ^* are in polar coordinates transformed to

$$\tau = -\mathrm{i}e^{\mathrm{i}\varphi}\partial_r + \frac{1}{r}e^{\mathrm{i}\varphi}\partial_\varphi, \quad \tau^* = -\mathrm{i}e^{-\mathrm{i}\varphi}\partial_r - \frac{1}{r}e^{-\mathrm{i}\varphi}\partial_\varphi. \tag{58}$$

Thus we solve equation

$$\tau^*\tau\psi = (-\partial_r^2 - \frac{1}{r}\partial_r - \frac{1}{r^2}\partial_\varphi^2)\psi = \lambda\psi \tag{59}$$

for ψ satisfying boundary conditions $\psi(r_1, \varphi) = 0$, $(\tau\psi)(r_2, \varphi) = 0$, $\psi(r, 0) = \psi(r, \alpha)$, $\partial_\varphi\psi(r, 0) = \partial_\varphi\psi(r, \alpha)$. We search for solutions in a separated form $\psi(r, \varphi) = \rho(r)\kappa(\varphi)$ and inserting the latter into (59), we get

$$\kappa(\varphi) = C_1 e^{-\mathrm{i}\sigma\varphi}, \quad \sigma = \frac{2\pi m}{\alpha}, \, m \in \mathbb{Z} \tag{60}$$

and ρ is the solution of

$$r^2\rho''(r) + r\rho'(r) + (\lambda r^2 - \sigma^2)\rho(r) = 0, \tag{61}$$

satisfying boundary conditions $\rho(r_1) = 0$ and $\rho'(r_2) + \frac{\sigma}{r_2}\rho(r_2) = 0$. This is similar to the situation encountered in the previous example, with the eigenfunctions separating into the exponential and the solution of a Dirichlet-Robin problem. This solution can be expressed as the following linear combination of Bessel functions

$$\rho(r) = C_2 J_\sigma(rk) + C_3 Y_\sigma(rk), \tag{62}$$

where $0 \leq \lambda = k^2$ and $\sigma \geq 0$. The boundary conditions now lead to the following transcendental eigenvalue equation

$$\frac{r_2 k}{\sigma} = \frac{J_\sigma(r_2k)Y_\sigma(r_1k) - J_\sigma(r_1k)Y_\sigma(r_2k)}{J_\sigma(r_1k)Y'_\sigma(r_2k) - J'_\sigma(r_2k)Y_\sigma(r_1k)}, \tag{63}$$

where primes denote the derivative with respect to the argument of the function. We remark that, for negative σ, Bessel functions of negative order should be used instead.

We can analyse the eigenvalue equation when σ converges to $-\infty$ in a similar fashion as was done in the rectangle case, *cf.* Proposition 12. However, calculations for the annulus are substantially more complex. With $\alpha = 2\pi$ and hence $\sigma_m = m$, we obtain

$$\lambda_{m,1} = \frac{-4m(1-m)}{r_2^2}\left(\frac{r_1}{r_2}\right)^{-2m} + \mathcal{O}\left(m^4 (r_1/r_2)^{-4m}\right) \tag{64}$$

and this expression remains valid for non-integer σ as well. Thus, as in the previous situation, we find a sequence of eigenvalues converging to zero exponentially when $\sigma \to -\infty$ and we can justify by similar arguments that the described eigenfunctions $\rho(r)\kappa(\varphi)$ form an orthonormal basis of $L^2(\Omega_{\mathrm{p}})$. ☐

Eigenfunctions corresponding to eigenvalues approaching zero localize to the boundary as in the example of the rectangle – see Figure 4.

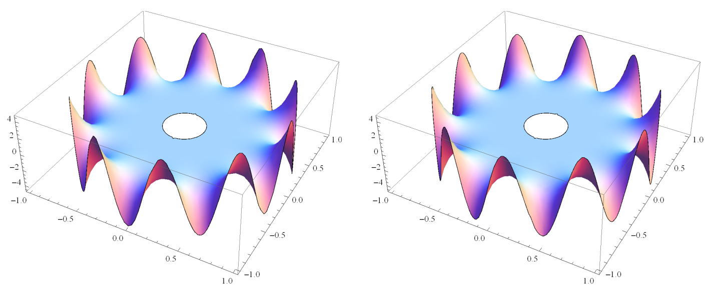

FIGURE 4. Real and imaginary part of $\psi_{-10,1}$ from Example 4.2 for $\alpha = 2\pi$, $r_1 = 0.2$, $r_2 = 1$.

As may be seen from the physics literature, *cf.* [1, 20], the boundary conditions in closed graphene systems are in fact of a more complex nature. More precisely, and following the approach in [1] for the case of a circular boundary, the zigzag boundary conditions should change as one moves around the boundary in the same way as for a regular hexagon. This way of modelling the boundary conditions for such situations was tested in [1] successfully against the numerical solution of the tight-binding model.

Thus, in the case of the annulus above, to obtain a physically relevant model the even and odd spinor components entering the zigzag boundary conditions (2) should be interchanged at angles which are multiples of $\pi/3$, while moving around the boundary, *i.e.*

$$\begin{aligned} &\forall \alpha \in (0,\pi/3)\cup(2\pi/3,\pi)\cup(4\pi/3,5\pi/3): &&\psi_1(r_1,\alpha)=0, &&\psi_3(r_1,\alpha)=0,\\ & &&\psi_2(r_2,\alpha)=0, &&\psi_4(r_2,\alpha)=0,\\ &\forall \alpha \in (\pi/3,2\pi/3)\cup(\pi,4\pi/3)\cup(4\pi/3,2\pi): &&\psi_2(r_1,\alpha)=0, &&\psi_4(r_1,\alpha)=0,\\ & &&\psi_1(r_2,\alpha)=0, &&\psi_3(r_2,\alpha)=0. \end{aligned} \tag{65}$$

Taking the square of the corresponding Dirac operator leads to Laplacians with combinations of Dirichlet and (anti-)Cauchy-Riemann boundary conditions, which is no longer an explicitly solvable spectral problem.

Nevertheless, our theoretical approach can be generalized to this situation in a straightforward way (we have to deal with a combination of the A and B operator types). In particular, the existence of a portion of the boundary where the Dirichlet boundary condition is imposed again prevents zero from being an eigenvalue, *cf.* the proof of Proposition 5, while the Dirichlet bracketing argument, *cf.* the proof of Proposition 6, shows that 0 is in the essential spectrum. Similar reasoning applies also for curved armchair-zigzag waveguides – see the remarks in Section 6.

4.3. **Rectangle with armchair and periodic boundary conditions.** As we saw in the previous sections, the behaviour for armchair boundary conditions is quite different, since we usually obtain "standard" operators defined in $W^{1,2}$. Write $\Omega := (-a,a) \times (-b,b)$ and define the operator in $L^2(\Omega, \mathbb{C}^4)$ by

$$
\begin{aligned}
H_{\mathrm{ap}}\Psi &:= H\Psi, \\
\mathrm{Dom}\,(H_{\mathrm{ap}}) &:= \big\{\Psi \in W^{1,2}(\Omega,\mathbb{C}^4) : \Psi_i \restriction \partial\Omega_3 = \Psi_{i+2} \restriction \partial\Omega_3, \\
&\qquad \Psi_i \restriction \partial\Omega_4 = e^{\mathrm{i}\Theta}\Psi_{i+2} \restriction \partial\Omega_4, \Psi_j \restriction \partial\Omega_1 = \Psi_j \restriction \partial\Omega_2 \\
&\qquad (i = 1,2,\ j = 1,...,4)\big\},
\end{aligned}
\tag{66}
$$

where $\partial_i\Omega$ are as in (36) and $\Theta \in \mathbb{R}$ is a physical parameter, *i.e.* we impose the combination of the armchair and periodic boundary conditions. The self-adjointness of this operator is discussed in the remark below Proposition 1. Further we study the spectrum of $H^2_{\mathrm{ap}} = \mathrm{diag}\{-\Delta,-\Delta,-\Delta,-\Delta\}$ with the domain $\mathrm{Dom}\,(H^2_{\mathrm{ap}}) = \{\Psi \in W^{2,2}(\Omega,\mathbb{C}^4) : \Psi_j \restriction \partial\Omega_1 = \Psi_j \restriction \partial\Omega_2, \partial_2\Psi_j \restriction \partial\Omega_1 = \partial_2\Psi_j \restriction \partial\Omega_2, \Psi_i \restriction \partial\Omega_3 = \Psi_{i+2} \restriction \partial\Omega_3, \Psi_i \restriction \partial\Omega_4 = e^{\mathrm{i}\Theta}\Psi_{i+2} \restriction \partial\Omega_4, \partial_1\Psi_i \restriction \partial\Omega_3 = -\partial_1\Psi_{i+2} \restriction \partial\Omega_3, \partial_1\Psi_i \restriction \partial\Omega_4 = -e^{\mathrm{i}\Theta}\partial_1\Psi_{i+2} \restriction \partial\Omega_4\ (i = 1,2,\ j = 1,\dots,4)\}$. We remark that the spectral problem corresponding to H_{ap} was studied directly in a formal way in [3, 27].

Proposition 15. *The spectrum of H^2_{ap} is discrete with eigenvalues given by $\lambda_{m,n} = \sigma_m^2 + \zeta_n^2$, $m,n \in \mathbb{Z}$, where $\sigma_m = m\pi/b$ and $\zeta_n = n\pi/(2a) - \Theta/(4a)$. The associated eigenfunctions*

$$
\Psi_{m,n} = e^{\mathrm{i}\sigma_m x_2}\begin{pmatrix} A_1 e^{-\mathrm{i}\zeta_n x_1} \\ C_1 e^{-\mathrm{i}\zeta_n x_1} \\ A_1(-1)^n e^{-\mathrm{i}\frac{\Theta}{2}} e^{\mathrm{i}\zeta_n x_1} \\ C_1(-1)^n e^{-\mathrm{i}\frac{\Theta}{2}} e^{\mathrm{i}\zeta_n x_1} \end{pmatrix},
\tag{67}
$$

where A_1, C_1 are normalization constants, form an orthonormal basis of $L^2(\Omega,\mathbb{C}^4)$.

Proof. Since calculations are standard we give only a brief description. Clearly, we can separate the even and odd components of Ψ and reduce the problem to two components of Ψ. It follows that the eigenfunctions are of the form $(\Psi_{m,n})_j(x_1,x_2) = e^{\mathrm{i}\sigma x_2}\kappa_j(x_1)$ $(j = 1,3)$, where $\kappa_j(x_1) = A_j e^{-\mathrm{i}\zeta x_1} + B_j e^{\mathrm{i}\zeta x_1}$. The latter must satisfy

$$
\kappa_1(-a) = \kappa_3(-a), \quad \kappa_1'(a) = -e^{\mathrm{i}\Theta}\kappa_3'(a).
\tag{68}
$$

This leads to the algebraic equation $\cos(4a\zeta) = \cos\Theta$ yielding solutions ζ_n. The eigenfunctions of this subproblem are κ_i with $A_1 \in \mathbb{C}$, $B_3 = A_1(-1)^n e^{-\mathrm{i}\Theta/2}$, $A_3 = B_1 = 0$, denoted by $\kappa_i^{(n)}$. Since $(\kappa_1^{(n)}, \kappa_3^{(n)})$ are the eigenfunctions of $\mathrm{diag}\{-\partial_1^2, -\partial_1^2\}$ defined on the functions from $W^{2,2}((-a,a),\mathbb{C}^2)$ satisfying the boundary conditions (68), in other words, they are eigenfunctions of a self-adjoint operator with a compact resolvent (an example of a quantum graph), they form an orthonormal basis of $L^2((-a,a),\mathbb{C}^2)$. Due to the structure of $\Psi_{m,n}$, the latter form an orthonormal basis of $L^2(\Omega,\mathbb{C}^4)$. □

4.4. **Rectangle with armchair and zigzag boundary conditions.** The combination of the zigzag and armchair boundary conditions is the most relevant physical situation, as it will be natural for some of the boundary lines to be at angles which are not compatible with both having one single type of boundary conditions. We intend to realize H, *cf.* (1), in $L^2(\Omega,\mathbb{C}^4)$ with $\Omega := (-a,a)\times(-b,b)$ as a self-adjoint operator and investigate the spectrum of its square. Formal calculations directly for the Dirac operator can be found in [26]. We start with a symmetric operator defined on C^1 functions satisfying boundary conditions,

$$\begin{aligned}
&\dot{H}_{\mathrm{az}}\Psi := H\Psi,\\
&\mathrm{Dom}\,(\dot{H}_{\mathrm{az}}) := \big\{\Psi \in C^1(\overline{\Omega}) : \Psi_i \restriction \partial\Omega_3 = \Psi_{i+2} \restriction \partial\Omega_3,\\
&\qquad \Psi_i \restriction \partial\Omega_4 = e^{\mathrm{i}\Theta}\Psi_{i+2} \restriction \partial\Omega_4,\\
&\qquad \Psi_j \restriction \partial\Omega_1 = 0, \Psi_{j+1} \restriction \partial\Omega_2 = 0 \ (i = 1,2,\ j = 1,3)\big\},
\end{aligned} \tag{69}$$

where $\partial_i\Omega$ are as in (36). We derive one inclusion of the closure of $\dot{H}_{\mathrm{az}}$.

Lemma 16. $\mathrm{Dom}\,(\overline{\dot{H}_{\mathrm{az}}}) \subset \mathscr{D}_{\mathrm{az}}$, *where* $\mathscr{D}_{\mathrm{az}} := \{\Psi \in L^2(\Omega,\mathbb{C}^4) : \Psi_j \in W^{1,2}_{\mathrm{loc}}(\overline{\Omega} \setminus \overline{\partial\Omega_2}), \Psi_{j+1} \in W^{1,2}_{\mathrm{loc}}(\overline{\Omega} \setminus \overline{\partial\Omega_1}), \Psi_i \restriction \partial\Omega_3 = \Psi_{i+2} \restriction \partial\Omega_3, \Psi_i \restriction \partial\Omega_4 = e^{\mathrm{i}\Theta}\Psi_{i+2} \restriction \partial\Omega_4, \Psi_j \restriction \partial\Omega_1 = 0, \Psi_{j+1} \restriction \partial\Omega_2 = 0 \ (i = 1,2,\ j = 1,3), H\Psi \in L^2(\Omega,\mathbb{C}^4)\}$

Proof. Let $\Psi \in \mathrm{Dom}\,(\overline{\dot{H}_{\mathrm{az}}})$, then there exists a sequence of functions Ψ_n from $\mathrm{Dom}\,(\dot{H}_{\mathrm{az}})$ such that $\Psi_n \to \Psi$ and $H\Psi_n \to \overline{\dot{H}}_{\mathrm{az}}\Psi$. Since the boundary conditions do not mix odd and even components, we restrict ourselves to the odd components only, *i.e.* we assume that $\Psi_2 = \Psi_4 = 0$.

For $\varepsilon > 0$, we take a real $C^1((-b,b))$ function $\xi_\varepsilon : [-b,b] \to [0,1]$ such that $\xi_\varepsilon = 1$ at $[-b, b-\varepsilon]$, $\xi_\varepsilon = 0$ at $[b-\varepsilon/2, b]$ and we define $\xi(x_1,x_2) := \xi_\varepsilon(x_2)$. Functions $\xi\Psi_n$ belong to $\mathrm{Dom}\,(\dot{H}_{\mathrm{az}})$, $\xi\Psi_n \to \xi\Psi$, and $\dot{H}_{\mathrm{az}}(\xi\Psi_n) \to \overline{\dot{H}}_{\mathrm{az}}(\xi\Psi)$. By partial integration, the graph norm of $\xi\Psi_n$ is equal to the $W^{1,2}$ norm, therefore $\xi\Psi \in W^{1,2}(\Omega,\mathbb{C}^4)$, satisfies the same boundary conditions as $\xi\Psi_n$, and $\overline{\dot{H}}_{\mathrm{az}}\Psi = H_{\mathrm{az}}\Psi$. ☐

We investigate further the eigenvalues and eigenfunctions of $\dot{H}^2_{\mathrm{az}}$ and we show that the latter form an orthonormal basis. It follows that $\dot{H}^2_{\mathrm{az}}$ is essentially self-adjoint. It is then not difficult to obtain eigenvalues and eigenfunctions of $\dot{H}_{\mathrm{az}}$, similarly as in Lemma 13 for zigzag and periodic boundary conditions, and conclude that $\dot{H}_{\mathrm{az}}$ is also essentially self-adjoint.

Proposition 17. *The eigenvalues of* $\dot{H}^2_{\mathrm{az}}$ *can be expressed as* $\lambda_{m,n} = \zeta_m^2 + \omega_{m,n}^2$, $m \in \mathbb{Z}$, $n \in \mathbb{N}$, *where* $\zeta_m = m\pi/(2a) - \Theta/(4a)$ *and* $\omega^2_{m,n}$ *are eigenvalues of the one-dimensional Dirichlet-Robin problems (indexed by* n *in increasing order)*

$$\begin{cases} -\xi_1'' = \omega^2_{m,n}\xi_1 & \text{in } (-b,b),\\ \xi_1 = 0 & \text{at } -b,\\ \xi_1' - \zeta_m\xi_1 = 0 & \text{at } b, \end{cases} \qquad \begin{cases} -\xi_2{}'' = \omega^2_{m,n}\xi_2 & \text{in } (-b,b),\\ \xi_2' + \zeta_m\xi_2 = 0 & \text{at } -b,\\ \xi_2 = 0 & \text{at } b, \end{cases} \tag{70}$$

i.e. $\omega^2_{m,n}$ *can be obtained from the solutions of the equation*

$$\zeta_m \sin(2\omega b) = \omega\cos(2\omega b). \tag{71}$$

Moreover,

$$\lim_{m\to+\infty} \zeta_m^2 + \omega^2_{m,1} = 0. \tag{72}$$

Associated eigenfunctions read

$$\Psi_{m,n}(x_1,x_2) = \begin{pmatrix} A_1 e^{-\mathrm{i}\zeta_m x_1}\sin(\omega_{m,n}(x_2+b))\\ C_1 e^{-\mathrm{i}\zeta_m x_1}\sin(\omega_{m,n}(x_2-b))\\ A_1(-1)^m e^{-\mathrm{i}\frac{\Theta}{2}} e^{\mathrm{i}\zeta_m x_1}\sin(\omega_{m,n}(x_2+b))\\ C_1(-1)^m e^{-\mathrm{i}\frac{\Theta}{2}} e^{\mathrm{i}\zeta_m x_1}\sin(\omega_{m,n}(x_2-b)) \end{pmatrix}, \tag{73}$$

where A_1, C_1 *are normalization constants, and they form an orthonormal basis of* $L^2(\Omega,\mathbb{C}^4)$.

Proof. As in the armchair-periodic case, *cf.* Proposition 15, we can separate the even and odd components of Ψ, therefore we focus only on odd ones further. The even ones can be examined in an analogous way, nonetheless, we remark that it follows from the symmetry that eigenvalues of both problems (70) coincide.

We search for solutions of $\dot{H}_{\mathrm{az}}^2\Psi = \lambda\Psi$ in a separated form, *i.e.* $\Psi_i = 0$ $(i = 2,4)$ and $\Psi_i(x_1,x_2) = \kappa_i(x_1)\xi_i(x_2)$ $(i = 1,3)$, where we take as κ_i those from Proposition 15, *i.e.* $\kappa_1^{(m)}(x_1) = A_1 e^{-\mathrm{i}\zeta_m x_1}$, $\kappa_3^{(m)}(x_1) = A_1(-1)^m e^{-\mathrm{i}\Theta/2}e^{\mathrm{i}\zeta_m x_1}$ with $\zeta_m = m\pi/(2a) - \Theta/(4a)$. This choice implies that $\xi_1 = \xi_3$ and ξ_1 is a solution of the Dirichlet-Robin problem (70). The latter is very similar to (42) from Proposition 12, the difference is the substitution of σ_m by ζ_m. The existence of a sequence of eigenvalues converging to zero and completeness of $\{\xi_1^{(m,n)}\}_{n\in\mathbb{N}}$ in $L^2((-b,b))$ for every m can be justified by the same arguments as in Proposition 12. The completeness of eigenfunctions $\Psi_{m,n}$ follows from the mentioned completeness of $\{\xi_1^{(m,n)}\}_{n\in\mathbb{N}}$ and the fact that $(\kappa_1^{(m)},0,\kappa_3^{(m)},0)$ together with $(0,\kappa_2^{(m)},0,\kappa_4^{(m)})$ form an orthonormal basis in $L^2((-a,a),\mathbb{C}^4)$. □

Finally, we can verify by straightforward calculations that eigenfunctions of $\dot{H}_{\mathrm{az}}$ have the following form.

Lemma 18. $\sigma_{\mathrm{p}}(\dot{H}_{\mathrm{az}}) = \{\pm\sqrt{\lambda_{m,n}}\}_{m\in\mathbb{Z},\,n\in\mathbb{N}}$. *The eigenfunctions corresponding to* $\pm\sqrt{\lambda_{m,n}}$ *read respectively:*

$$\Phi_{m,n}^{\pm}(x_1,x_2) = A_{m,n}^{\pm}\begin{pmatrix} \mp e^{-\mathrm{i}\zeta_m x_1}\sin(\omega_{m,n}(x_2+b)) \\ e^{-\mathrm{i}\zeta_m x_1}\sin(\omega_{m,n}(x_2-b)) \\ \mp(-1)^m e^{-\mathrm{i}\frac{\Theta}{2}}e^{\mathrm{i}\zeta_m x_1}\sin(\omega_{m,n}(x_2+b)) \\ (-1)^m e^{-\mathrm{i}\frac{\Theta}{2}}e^{\mathrm{i}\zeta_m x_1}\sin(\omega_{m,n}(x_2-b)) \end{pmatrix}, \tag{74}$$

and form an orthonormal basis of $L^2(\Omega,\mathbb{C}^4)$.

5. Waveguides

We shall now consider the case of waveguides, *i.e.* when the set Ω is an infinite strip such as $\Omega = \mathbb{R}\times(-a,a)$, for instance. Our analysis will be based on the above study when the operators were defined on rectangles, with periodic and either zigzag and armchair boundary conditions. These examples will be used to construct suitable singular sequences to investigate essential spectra of waveguide systems and we shall consider three physically relevant situations, *i.e.* the straight armchair waveguide and both straight and curved zigzag waveguides.

5.1. **Straight armchair waveguide.** Let $\Omega = \Omega_2 \equiv (-a,a)\times\mathbb{R}$ and define $H_{\mathrm{ac}}^{\mathrm{sw}} := H_{\mathrm{ac}}$, *cf.* Proposition 1. Since the domain of $H_{\mathrm{ac}}^{\mathrm{sw}}$ is a standard Sobolev space and $(H_{\mathrm{ac}}^{\mathrm{sw}})^2$ can be written as a sum of a longitudinal and transverse operator $-\partial_2^2$ and $-\partial_1^2$ respectively with appropriate boundary conditions, the following result on the spectrum of the waveguide is very natural.

Proposition 19. $\sigma(H_{\mathrm{ac}}^{\mathrm{sw}}) = \sigma_{\mathrm{ess}}(H_{\mathrm{ac}}^{\mathrm{sw}}) = (-\infty,-E_0]\cup[E_0,\infty)$, *where* $E_0 := \min_{n\in\mathbb{Z}}|\zeta_n|$ *with* $\zeta_n = n\pi/(2a) - \Theta/(4a)$, cf. *Section 4.3 and, in particular, Proposition 15.*

Proof. Let ζ_{n_0} be such that $E_0 = |\zeta_{n_0}|$. The singular sequence for $\lambda\in[E_0,\infty)$, to be inserted into the Weyl criterion, can be expressed as

$$\Psi_\lambda^{(n)}(x_1,x_2) := e^{\mathrm{i}\sigma x_2}\frac{\psi_n(x_2)}{\|\psi_n\|_{L^2(\mathbb{R})}}\begin{pmatrix} e^{-\mathrm{i}\zeta_{n_0}x_1} \\ \frac{-\zeta_{n_0}+\mathrm{i}\sigma}{\sqrt{\zeta_{n_0}^2+\sigma^2}}e^{-\mathrm{i}\zeta_{n_0}x_1} \\ (-1)^{n_0}e^{-\mathrm{i}\frac{\Theta}{2}}e^{\mathrm{i}\zeta_{n_0}x_1} \\ (-1)^{n_0}e^{-\mathrm{i}\frac{\Theta}{2}}\frac{-\zeta_{n_0}+\mathrm{i}\sigma}{\sqrt{\zeta_{n_0}^2+\sigma^2}}e^{\mathrm{i}\zeta_{n_0}x_1} \end{pmatrix}, \tag{75}$$

where $n \in \mathbb{N}$, σ is such that $\lambda = \sqrt{\sigma^2 + \zeta_{n_0}^2}$ and $\psi_n(x_2) := \phi(x_2/n - n)$ with $\phi(x_2) \in C_0^\infty((-1,1))$. Properties of ψ_n imply that $\Psi^{(n)}/\|\Psi_\lambda^{(n)}\| \xrightarrow{\mathrm{w}} 0$. Moreover, it can be verified that $\|(H_{\mathrm{ac}}^{\mathrm{sw}} - \lambda)\Psi_\lambda^{(n)}\|/\|\Psi_\lambda^{(n)}\| \to 0$. A similar singular sequence can be constructed for $\lambda \in (-\infty, E_0]$ by multiplying the even components of $\Psi_\lambda^{(n)}$ by -1.

To justify that no point in $(-E_0, E_0)$ is in the spectrum, we can consider $(H_{\mathrm{ac}}^{\mathrm{sw}})^2$ and, by standard arguments for tensor products [21, Thm.VIII.33], show that $\sigma((H_{\mathrm{ac}}^{\mathrm{sw}})^2) = [E_0^2, \infty)$. □

We note that armchair boundary conditions seem to be relevant only for straight strips in particular directions, while most other configurations such as curved strips are generically described by zigzag boundary conditions, see *e.g.* [1].

5.2. **Straight and curved zigzag waveguides.** Unlike in the armchair case where, depending on Θ, there is a gap in the essential spectrum around zero, the essential spectrum of zigzag waveguides covers the whole real line. This is what is to be expected from the operator H_{zp} defined on a rectangle where the zigzag boundary conditions where complemented with periodic boundary conditions. Using a standard approach in quantum waveguide literature [9, 18], we show that the essential spectra of both straight and asymptotically straight zigzag waveguides cover the whole $\mathbb{R}$ by means of the Weyl criterion directly for the operator H_{zp}; we insert singular sequences having the form of (56) with suitable modifications.

We begin by considering the straight waveguide, *i.e.* $\Omega = \Omega_1 \equiv \mathbb{R} \times (-b, b)$. We denote $\partial\Omega^1 := \mathbb{R} \times \{-b\}$, $\partial\Omega^2 := \mathbb{R} \times \{b\}$ and define the following operator in $L^2(\Omega, \mathbb{C}^2)$

$$
\begin{aligned}
&H_{\mathrm{zz}}^{\mathrm{sw}}\Psi := H_1\Psi, \\
&\mathrm{Dom}\,(H_{\mathrm{zz}}^{\mathrm{sw}}) := \big\{\Psi \in L^2(\Omega, \mathbb{C}^2) : \Psi_i \in W_{\mathrm{loc}}^{1,2}(\Omega \cup \partial\Omega^i), \Psi \restriction \partial\Omega^i = 0 \\
&\qquad (i = 1,2), H_1\Psi \in L^2(\Omega, \mathbb{C}^2)\big\},
\end{aligned}
\tag{76}
$$

where the notation is similar as that of Proposition 3, *i.e.* $\Psi_i \in W_{\mathrm{loc}}^{1,2}(\Omega \cup \partial\Omega^i)$ if $\Psi_i \in W^{1,2}(\Omega')$ for any $\Omega' \subset \Omega$ such that $\overline{\Omega'} \subset \Omega \cup \partial\Omega^i$. A modification of the proof of that proposition yields that $H_{\mathrm{zz}}^{\mathrm{sw}}$ is self-adjoint.

Proposition 20. $\sigma_{\mathrm{ess}}(H_{\mathrm{zz}}^{\mathrm{sw}}) = \mathbb{R}$.

Proof. We consider the sequence

$$
\Psi_{-\sqrt{\lambda}}^{(n)}(x_1, x_2) := e^{-\mathrm{i}\sigma x_1} \frac{\psi_n(x_1)}{\|\psi_n\|_{L^2(\mathbb{R})}} \begin{pmatrix} \sin(\omega(x_2 + a)) \\ \sin(\omega(x_2 - a)) \end{pmatrix} \equiv \Psi^{(n)}(x_1, x_2)
\tag{77}
$$

where $\sigma \sin(2\omega a) = \omega \cos(2\omega a)$, $\lambda = \sigma^2 + \omega^2$, and $\psi_n(x_1) := \phi(x_1/n - n)$ with $\phi(x_1) \in C_0^\infty((-1,1))$. The relation between σ and ω in fact corresponds to the eigenvalue equation on the rectangle with periodic boundary conditions, *cf.* (43), although the "quantization" of σ is relaxed here.

Clearly $\|\Psi^{(n)}\|$ is bounded and does not depend on n. Moreover, $\Psi^{(n)} \xrightarrow{\mathrm{w}} 0$ because of the properties of ψ_n. We start with the identity

$$
\|(H_{\mathrm{zz}}^{\mathrm{sw}} + \sqrt{\lambda})\Psi^{(n)}\|^2 = \|\tau\Psi_1^{(n)} + \sqrt{\lambda}\,\Psi_2^{(n)}\|_{L^2(\mathbb{R})}^2 + \|\tau^*\Psi_2^{(n)} + \sqrt{\lambda}\,\Psi_1^{(n)}\|_{L^2(\mathbb{R})}^2,
\tag{78}
$$

of which we analyse only the first term on the right–hand side in detail.

$$
\begin{aligned}
\tau\Psi_1^{(n)} + \sqrt{\lambda}\,\Psi_2^{(n)} &= e^{-\mathrm{i}\sigma x_1}\big(- \sigma \sin(\omega(x_2+a)) + \omega\cos(\omega(x_2+a)) \\
&\quad + \sqrt{\lambda}\sin(\omega(x_2-a))\big)\frac{\psi_n(x_1)}{\|\psi_n\|_{L^2(\mathbb{R})}} \\
&\quad - \mathrm{i}e^{-\mathrm{i}\sigma x_1}\sin(\omega(x_2+a))\frac{\psi_n'(x_1)}{\|\psi_n\|_{L^2(\mathbb{R})}}.
\end{aligned} \tag{79}
$$

Inserting the relations between σ, ω and λ, we find that

$$
-\sigma\sin(\omega(x_2+a)) + \omega\cos(\omega(x_2+a)) + \sqrt{\lambda}\sin(\omega(x_2-a) = 0. \tag{80}
$$

Therefore (78) reduces to

$$
\begin{aligned}
&\|(H_{\mathrm{zz}}^{\mathrm{sw}} + \sqrt{\lambda})\Psi^{(n)}\|^2 = \\
&\Big(\|\sin(\omega(x_2+a))\|^2_{L^2((-a,a))} + \|\sin(\omega(x_2-a))\|^2_{L^2((-a,a))}\Big)\frac{\|\psi_n'\|^2_{L^2(\mathbb{R})}}{\|\psi_n\|^2_{L^2(\mathbb{R})}}.
\end{aligned} \tag{81}
$$

Since $\|\psi_n'\|_{L^2(\mathbb{R})}/\|\psi_n\|_{L^2(\mathbb{R})} = C/n$ with C depending only on ϕ, the point $-\sqrt{\lambda}$ belongs to the essential spectrum of $H_{\mathrm{zz}}^{\mathrm{sw}}$. Using the symmetry, as in Lemma 13, we can construct a singular sequence for $\sqrt{\lambda}$ as well.

We remark that relations between σ, ω and λ can be rewritten in the following way (for $2\omega a \neq n\pi$)

$$
\sigma = \omega\cot(2\omega a), \quad \sqrt{\lambda} = \frac{|\omega|}{|\sin(2\omega a)|}. \tag{82}
$$

For $\omega \in (0, \pi/(2a))$ we obtain $(1/(2a), +\infty)$ for the range of $\sqrt{\lambda}$ while taking $-\mathrm{i}\omega \in (0,\infty)$ yields the remaining $(0, 1/(2a))$. □

We shall now introduce a curved waveguide similarly as in [9], referring to [18] for an extensive discussion on this issue. We take Ω as a curved planar strip, *i.e.* $\Omega := \{(x,y) \in \mathbb{R}^2 : x = a(s) - ub'(s), y = a(s) + ub'(s), s \in \mathbb{R}, u \in (-b,b)\}$, determined by the reference curve $\Gamma := \{(a(s), b(s)) : s \in \mathbb{R}\}$ and denote by $\partial\Omega^i$ $(i = 1,2)$ the lower and upper parts of the boundary, respectively. It is assumed that $a'(s)^2 + b'(s)^2 = 1$, *i.e.* Γ is parametrized by arclenght and we denote by γ the signed curvature of Γ, *i.e.* $\gamma(s) = b'(s)a''(s) - a'(s)b''(s)$. We further assume that γ is continuous, $2b\|\gamma\|_\infty < 1$, and the curved waveguide Ω obtained is not self-intersecting, *cf.* [9, 18] for further details. If the curvature of the reference curve vanishes at infinity, *i.e.* $\gamma(s) \to 0$ as $s \to \pm\infty$, the waveguide is called asymptotically straight.

The operator $H_{\mathrm{zz}}^{\mathrm{cw}}$ corresponding to the curved waveguide is defined in $L^2(\Omega, \mathbb{C}^2)$ by

$$
\begin{aligned}
&H_{\mathrm{zz}}^{\mathrm{cw}}\Psi := H_1\Psi, \\
&\mathrm{Dom}\,(H_{\mathrm{zz}}^{\mathrm{cw}}) := \big\{\Psi \in L^2(\Omega, \mathbb{C}^2) : \Psi_i \in W^{1,2}_{\mathrm{loc}}(\Omega \cup \partial\Omega^i), \Psi \restriction \partial\Omega^i = 0 \\
&\qquad\qquad (i = 1,2), H_1\Psi \in L^2(\Omega, \mathbb{C}^2)\big\},
\end{aligned} \tag{83}
$$

where the function space notation is introduced above for the straight waveguide. A modification of the proof of Proposition 3 yields that $H_{\mathrm{zz}}^{\mathrm{cw}}$ is self-adjoint.

The essential spectrum of curved zigzag waveguide remains unchanged as was to be expected from what happens to usual quantum waveguides.

Proposition 21. *Let $\gamma(s) \to 0$ as $s \to \pm\infty$, then $\sigma_{\mathrm{ess}}(H_{\mathrm{zz}}^{\mathrm{cw}}) = \mathbb{R}$.*

Proof. The idea of the proof runs along the lines of the standard approach for quantum waveguides [9, 18] and we use a modification of the singular sequence used in the straight case. We first write the differential expressions τ and τ^* in curvilinear coordinates (s, u)

$$\tau = e^{-\mathrm{i}\varphi(s)}(-\mathrm{i}f^{-1}(s,u)\partial_s + \partial_u), \quad \tau^* = e^{\mathrm{i}\varphi(s)}(-\mathrm{i}f^{-1}(s,u)\partial_s - \partial_u), \tag{84}$$

where $f(s, u) := 1 + u\gamma(s)$ and $e^{\mathrm{i}\varphi(s)} = a'(s) - \mathrm{i}b'(s)$ from which it follows that $\varphi' = \gamma$. This change of coordinates also implies that we change the Hilbert space from $L^2(\Omega, \mathbb{C}^2)$ to $L^2(\Omega_0, \mathbb{C}^2, f\mathrm{d}s\mathrm{d}u)$, where $\Omega_0 := \mathbb{R}\times(-b, b)$. We denote the norm in the new space by $\|\cdot\|_0$. We shall now define the sequence

$$\Psi^{(n)}_{-\sqrt{\lambda}}(s,u) := e^{-\mathrm{i}\sigma s}\frac{\psi_n(s)}{\|\psi_n\|_{L^2(\mathbb{R})}}\begin{pmatrix} e^{\mathrm{i}\frac{\varphi(s)}{2}}\sin(\omega(u+b)) \\ e^{-\mathrm{i}\frac{\varphi(s)}{2}}\sin(\omega(u-b)) \end{pmatrix} \equiv \Psi^{(n)}(s,u), \tag{85}$$

where $\psi_n(s) := \phi(s/n - n)$ with $\phi(s) \in C_0^\infty((-1, 1))$ and, as in the straight case, $\sigma \sin(2\omega a) = \omega \cos(2\omega a)$, $\lambda = \sigma^2 + \omega^2$. We insert this sequence into Weyl criterion

$$\|(H^{\mathrm{cw}}_{\mathrm{zz}} + \sqrt{\lambda})\Psi^{(n)}\|_0^2 = \|(\tau\Psi^{(n)}_1 + \sqrt{\lambda}\,\Psi^{(n)}_2)\|_0^2 + \|(\tau^*\Psi^{(n)}_2 + \sqrt{\lambda}\,\Psi^{(n)}_1)\|_0^2, \tag{86}$$

and analyse only the first term in detail.

$$\begin{aligned} \tau\Psi^{(n)}_1 + \sqrt{\lambda}\,\Psi^{(n)}_2 = e^{-\mathrm{i}\frac{\varphi(s)}{2}}\bigg(& (-\mathrm{i}\partial_s + \partial_u)e^{-\mathrm{i}\sigma s}\frac{\psi_n(s)}{\|\psi_n\|_{L^2(\mathbb{R})}}\sin(\omega(u+b)) \\ & + \sqrt{\lambda}e^{-\mathrm{i}\sigma s}\frac{\psi_n(s)}{\|\psi_n\|_{L^2(\mathbb{R})}}\sin(\omega(u-b))\bigg) \\ & + \mathrm{i}e^{-\mathrm{i}\frac{\varphi(s)}{2}}\frac{u\gamma(s)}{f(s,u)}\partial_s(e^{-\mathrm{i}\sigma s}\psi_n(s))\frac{\sin(\omega(u+b))}{\|\psi_n\|_{L^2(\mathbb{R})}} \\ & + \mathrm{i}e^{-\mathrm{i}\frac{\varphi(s)}{2}}\frac{\gamma(s)}{2f(s,u)}e^{-\mathrm{i}\sigma s}\frac{\psi_n(s)}{\|\psi_n\|_{L^2(\mathbb{R})}}\sin(\omega(u+b)), \end{aligned} \tag{87}$$

where we used the definition of f and $\varphi' = \gamma$. The norm of the first term at r.h.s tends to zero as $n \to +\infty$ for the same reason as in the straight case, while the other terms tend to zero because the support of ψ_n "escapes" to infinity and $\gamma(s) \to 0$ as $s \to \pm\infty$. □

6. Concluding remarks

The spectra of graphene nanorribons are highly sensitive to the different types of boundary conditions which, in turn, depend on the orientation of the boundary with respect to the graphene lattice. As we have shown, zigzag boundary conditions necessarily lead to a non-empty essential spectrum resulting in the existence of edge states with energies converging to zero exponentially. From the mathematical point of view, the properties of edge states, namely the localization at the boundary and zero being the accumulation point of energies, are a consequence of local compactness of the resolvent. In the presence of a potential, the essential spectrum is moved depending on the values of the potential at the boundary where zigzag boundary conditions are imposed. Besides perturbations by a potential V, the addition of a magnetic field or, more generally, off-diagonal perturbations, coming for instance from a non-trivial geometry of the manifolds or deformations of the atom lattice and which have appeared frequently in the literature for various graphene configurations (*e.g.* planar sheets, nanotubes), see *e.g.* [5, 25, 15, 14], deserves further study. The practical interest in the addition of the magnetic field lies in the possibility of opening the energy gap around zero in infinite graphene systems, for instance in infinite strips (waveguides), where the essential spectrum typically covers the whole real line.

An important issue that was considered only briefly in this work in Example 4.4, is the combination of armchair and zigzag boundary conditions. Such interfaces are known to have physical consequences *e.g.* in scattering [27]. In the context of curved graphene waveguides, the most interesting system should be a strip that is straight at both ends corresponding to the armchair edge and curved in a finite region where zigzag boundary conditions are prevalent. Based on our analysis, the essential spectrum (of the square of the Dirac operator) will contain $[E_0, \infty)$ coming from the infinite armchair parts, see Section 5.1, and zero due to the presence of the "zigzag region". The existence of a gap in the essential spectrum between zero and E_0 is to be expected, but this requires further analysis. The interesting features characteristic of quantum waveguides, namely the geometrically induced bound states below E_0, *cf.* [9], could then be studied in such systems as well. However, the *traditional* variational argument used in that setting cannot be applied here directly due to the unavoidable zero in the essential spectrum.

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