Operators and Matrices
Volume 14, Number 3 (2020), 667–678
doi:10.7153/oam-2020-14-42

SELF–ADJOINT EXTENSIONS OF THE TWO–VALLEY DIRAC OPERATOR WITH DISCONTINUOUS INFINITE MASS BOUNDARY CONDITIONS

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Abstract. We consider the four-component two-valley Dirac operator on a wedge in $\mathbb{R}^2$ with infinite mass boundary conditions, which enjoy a flip at the vertex. We show that it has deficiency indices $(1,1)$ and we parametrize all its self-adjoint extensions, relying on the fact that the underlying two-component Dirac operator is symmetric with deficiency indices $(0,1)$. The respective defect element is computed explicitly. We observe that there exists no self-adjoint extension, which can be decomposed into an orthogonal sum of two two-component operators. In physics, this effect is called *mixing the valleys*.

1. Introduction

The dynamics of low-energy electrons in graphene is effectively described by a Hamiltonian associated to the matrix differential expression

$$\mathscr{M} = \begin{pmatrix} \mathscr{D} & 0 \\ 0 & \mathscr{D} \end{pmatrix},$$

where $\mathscr{D}$ is the two-component Dirac differential expression in two dimensions. Such a Hamiltonian takes into account contributions from the two inequivalent Dirac points (or valleys) of the first Brillouin zone associated to the underlying hexagonal lattice. The respective components of a wavefunction describe the electronic density on each of the two triangular sublattices that constitute the honeycomb lattice. In order to define rigorously the operator associated to $\mathscr{M}$, appropriate boundary conditions have to be imposed, and its domain of self-adjointness has to be determined. In many applications the two valleys are decoupled and the description is reduced to the study of an operator associated to $\mathscr{D}$ only. However, interactions that mix the valleys may indeed occur in graphene [20] and the effects produced by them are often appearing under the name *valleytronics*; see [15] and the references therein. In this paper we consider a discontinuous *infinite mass* boundary condition and, in order to get self-adjointness for the operator associated to $\mathscr{M}$, it is necessary to couple the two valleys.

Mathematics subject classification (2010): 35P05, 35Q40, 81Q10.
Keywords and phrases: Dirac operator, infinite mass boundary condition, wedge, self-adjoint extensions, mixing the valleys.
The authors are grateful for the support by the grant No. 17-01706S of the Czech Science Foundation (GAČR). The research of first author is also supported by Fondo Sociale Europeo – Programma Operativo Nazionale Ricerca e Innovazione 2014-2020, progetto PON: progetto AIM1892920-attività 2, linea 2.1 - CUP H95G18000150006 ATT2.
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Following our program, we investigate the two-dimensional massless Dirac operator with discontinuous infinite mass boundary conditions on a wedge in the situation when the boundary condition undergoes a flip at the vertex. This problem can be regarded as a counterpart of the analysis in [11, 18] for a similar problem without a flip. Following the strategy of [11], in order to obtain the main result we rely on separation of the variables and subsequent careful analysis of the one-dimensional fiber operators. We would like to emphasize that the observed effect is essentially not caused by the corner of the wedge, because it persists even if the flip happens on the half-plane. In this respect it is reminiscent of a similar effect for the Robin Laplacian with the coefficient having a linear singularity at a boundary point [9, 12, 14]. We expect that relying on the localisation technique given in [14], our results can be generalized for operators on smooth planar domains and even on curvilinear polygons, having (finitely many) flips of the boundary condition. The literature on Dirac operators with infinite mass boundary conditions on domains is quite extensive; see *e.g.* [1, 2, 3, 5, 10, 17], the review papers [4, 16], and the references therein.

To describe our main result we need to introduce some notations. In what follows, we consider a wedge:

$$\mathscr{S}_\omega := \left\{(r\cos\theta, r\sin\theta)\in\mathbb{R}^2 \colon r>0, \theta\in\mathbb{I}_\omega\right\}\subset\mathbb{R}^2, \tag{1.1}$$

where $\mathbb{I}_\omega := (-\omega,\omega)$ with $\omega\in(0,\pi)$. The value 2ω can be viewed as the opening angle of the wedge $\mathscr{S}_\omega$. The opposite sides of the wedge $\mathscr{S}_\omega$ are denoted by

$$\Gamma_\omega^\pm := \left\{(r\cos\omega, \pm r\sin\omega)\in\mathbb{R}^2 \colon r>0\right\}.$$

Clearly, the choice $\omega=\frac{\pi}{2}$ corresponds to the half-plane.

Recall that the 2×2 Hermitian *Pauli matrices* $\sigma_1,\sigma_2,\sigma_3$ are given by

$$\sigma_1=\begin{pmatrix}0&1\\1&0\end{pmatrix},\qquad \sigma_2=\begin{pmatrix}0&-\mathrm{i}\\ \mathrm{i}&0\end{pmatrix}\quad\text{and}\quad \sigma_3=\begin{pmatrix}1&0\\0&-1\end{pmatrix}.$$

For $i,j\in\{1,2,3\}$, they satisfy the anti-commutation relation $\sigma_j\sigma_i+\sigma_i\sigma_j=2\delta_{ij}$, where δ_{ij} is the Kronecker symbol. For the sake of convenience, we define $\sigma:=(\sigma_1,\sigma_2)$ and for $x=(x_1,x_2)^\top\in\mathbb{R}^2$ we set

$$\sigma\cdot x := x_1\sigma_1+x_2\sigma_2=\begin{pmatrix}0 & x_1-\mathrm{i}x_2\\ x_1+\mathrm{i}x_2 & 0\end{pmatrix}.$$

Consider the following matrix differential expression

$$\mathscr{D} := -\mathrm{i}(\sigma\cdot\nabla)=\begin{pmatrix}0 & -\mathrm{i}(\partial_1-\mathrm{i}\partial_2)\\ -\mathrm{i}(\partial_1+\mathrm{i}\partial_2) & 0\end{pmatrix}.$$

The subject of our analysis is the Dirac operator D_ω in the Hilbert space $L^2(\mathscr{S}_\omega;\mathbb{C}^2)$, defined as follows:

$$\begin{aligned}
\mathsf{D}_\omega u &:= \mathscr{D}u,\\
\operatorname{dom}\mathsf{D}_\omega &:= \left\{u=\begin{pmatrix}u_1\\u_2\end{pmatrix}\in H^1(\mathscr{S}_\omega;\mathbb{C}^2)\colon \begin{matrix} u_2|_{\Gamma_\omega^+}=-e^{+\mathrm{i}\omega}u_1|_{\Gamma_\omega^+}\\ u_2|_{\Gamma_\omega^-}=-e^{-\mathrm{i}\omega}u_1|_{\Gamma_\omega^-}\end{matrix}\right\}.
\end{aligned}\tag{1.2}$$

Denoting $\mathbf{n} := \mathbf{n}(x)$ the outer unit normal at the point $x \in \partial\mathscr{S}_\omega \setminus \{0\} = \Gamma_\omega^- \cup \Gamma_\omega^+$, an explicit computation shows that the boundary conditions in (1.2) are equivalent to

$$u = \mp \mathrm{i}\sigma_3(\sigma\cdot\mathbf{n})u, \quad \text{on } \Gamma_\omega^\pm. \tag{1.3}$$

We remark that the standard realization of the Dirac operator on a wedge with infinite mass boundary conditions prescribes that

$$u = -\mathrm{i}\sigma_3(\sigma\cdot\mathbf{n})u, \quad \text{on } \partial\mathscr{S}_\omega,$$

while in (1.3) there is a flip between the boundary conditions imposed on the opposite sides $\Gamma_\omega^\pm$ of the wedge. Equivalently, in order to get standard infinite mass boundary conditions one should replace the second condition $u_2|_{\Gamma_\omega^-} = -e^{-\mathrm{i}\omega}u_1|_{\Gamma_\omega^-}$ in (1.2) by $u_2|_{\Gamma_\omega^-} = e^{-\mathrm{i}\omega}u_1|_{\Gamma_\omega^-}$.

We show in Proposition 2.1 that the operator D_ω is symmetric. Our first main result concerns the deficiency indices and subspaces of D_ω.

THEOREM 1.1. *Let the symmetric operator* D_ω *be as in* (1.2)*. Then the following properties hold:*

(i) D_ω *has deficiency indices* $(0,1)$.[1]

(ii) $\ker(\mathsf{D}_\omega^* + \mathrm{i}) = \mathrm{span}\{u_\star\}$ *and the defect element is given in polar coordinates by*

$$u_\star(r,\theta) = \frac{1}{2\sqrt{\omega}}\frac{e^{-r}}{\sqrt{r}}\begin{pmatrix} e^{-\frac{\mathrm{i}\theta}{2}} \\ -e^{\frac{\mathrm{i}\theta}{2}}\end{pmatrix}. \tag{1.4}$$

In order to prove Theorem 1.1, we take the advantage of the reformulation in polar coordinates: we decompose the operator D_ω into an orthogonal sum of infinitely many one-dimensional self-adjoint Dirac operators on the half-line and a momentum-type operator on the half-line, which has deficiency indices $(0,1)$ and whose defect element can be explicitly computed by solving an elementary first-order ODE.

The full four-component two-valley Dirac operator on a planar domain with infinite mass boundary conditions can be viewed as an orthogonal sum of two two-component (one-valley) Dirac operators with infinite mass boundary conditions, in which the unit normals are chosen to point outwards and inwards, respectively. As previously mentioned, the analysis reduces to the one-valley two-component Dirac operator unless there is an additional "off-diagonal" interaction, which mixes the valleys.

In our setting, the two-component Dirac operator associated with the first valley is precisely given by D_ω, while the one associated with the second valley

$$\left\{u = (u_1,u_2)^\top \in H^1(\mathscr{S}_\omega;\mathbb{C}^2) \colon u_2|_{\Gamma_\omega^\pm} = e^{\pm\mathrm{i}\omega}u_1|_{\Gamma_\omega^\pm}\right\} \ni u \mapsto \mathscr{D}u$$

[1] For $\mathsf{S} \subset \mathsf{S}^*$ we adopt the convention $n_+(\mathsf{S}) := \dim\ker(\mathsf{S}^* - \mathrm{i})$ and $n_-(\mathsf{S}) := \dim\ker(\mathsf{S}^* + \mathrm{i})$. The deficiency indices of S are given by $(n_+(\mathsf{S}), n_-(\mathsf{S}))$.

is unitarily equivalent to $-\mathsf{D}_\omega$ via the Pauli matrix σ_3. Hence, the two-valley Dirac operator is unitarily equivalent to

$$\mathsf{M}_\omega := \mathsf{D}_\omega \oplus (-\mathsf{D}_\omega). \tag{1.5}$$

Clearly, the operator M_ω is symmetric in $L^2(\mathscr{S}_\omega;\mathbb{C}^4)$.

Our second main result concerns the characterisation of the self-adjoint extensions for M_ω. In our model, mixing the valleys naturally enters as a necessity to define a self-adjoint Hamiltonian through the coupling constant $\alpha \in \mathbb{T}$, which parametrizes the extension. Moreover, this mixing is inevitable, since there is no self-adjoint extension of M_ω, which can be represented as an orthogonal sum of two Hamiltonians with respect to the decomposition $L^2(\mathscr{S}_\omega;\mathbb{C}^4) = L^2(\mathscr{S}_\omega;\mathbb{C}^2) \oplus L^2(\mathscr{S}_\omega;\mathbb{C}^2)$. This mathematical observation still awaits a thorough physical interpretation.

THEOREM 1.2. *Let the symmetric operator D_ω be as in (1.2) and let $u_\star$ be as in (1.4). Then the two-valley Dirac operator $\mathsf{M}_\omega = \mathsf{D}_\omega \oplus (-\mathsf{D}_\omega)$ has deficiency indices $(1,1)$ and all its self-adjoint extensions are given by*

$$\mathsf{M}_{\alpha,\omega} := \begin{pmatrix} \mathscr{D}u_1 + \mathrm{i}u_\star \\ -\mathscr{D}u_2 - \mathrm{i}\alpha u_\star \end{pmatrix},$$

$$\operatorname{dom} \mathsf{M}_{\alpha,\omega} := \left\{ \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} + \begin{pmatrix} u_\star \\ \alpha u_\star \end{pmatrix} : u_1, u_2 \in \operatorname{dom} \mathsf{D}_\omega \right\},$$

where $\alpha \in \mathbb{T} := \{z \in \mathbb{C} \colon |z| = 1\}$ is an extension parameter.

The proof of Theorem 1.2 rests upon Theorem 1.1 and classical von Neumann extensions theory; *cf* [19, §X.1].

REMARK 1. It is not yet clear if there is a way to single out a distinguished self-adjoint extension of M_ω. In this respect, the analysis of the case without a flip is different: the two-dimensional Dirac operator is essentially self-adjoint whenever $0 < \omega \leqslant \pi/2$ and for $\pi/2 < \omega < \pi$ it has a unique extension such that its domain is included in $H^{\frac{1}{2}}(\mathscr{S}_\omega;\mathbb{C}^2)$; *cf.* [11] for the infinite mass boundary condition and [18] for more general quantum-dot boundary conditions. In our case, Theorem 1.2 shows that the regularity of the operator domain can not be a criterion for selection, because it is impossible to single out an extension requiring that its domain is included in a Sobolev space $H^s(\mathscr{S}_\omega;\mathbb{C}^4)$, for some specific $s > 0$. Indeed, in our setting for any $0 < \omega < \pi$ all the extensions have a function in the domain that has a singularity $\sim |x|^{-\frac{1}{2}}$ at the origin. An analogous phenomenon was observed in [6, Rem. 1.10] and [7, Rem. 1.11] for Dirac operators with critical Coulomb-type spherically symmetric perturbations.

Organisation of the paper

We prove in Section 2 that the operator D_ω is symmetric and obtain its equivalent representation in polar coordinates. Then, we decompose the operator D_ω into orthogonal sum of one-dimensional fiber operators in Section 3. Finally, Theorems 1.1 and 1.2 are proven in Section 4.

2. Preliminary analysis of D_ω

2.1. Symmetry

In order to prove symmetry of D_ω we employ integration by parts. Thanks to the specific choice of the boundary condition, the boundary term vanishes.

We denote by $(\cdot,\cdot)_{\mathscr{S}_\omega}$ the inner product in $L^2(\mathscr{S}_\omega;\mathbb{C}^2)$. Note that all the inner products in the present paper are linear in the first entry.

PROPOSITION 2.1. *The operator D_ω is densely defined and symmetric in the Hilbert space $L^2(\mathscr{S}_\omega;\mathbb{C}^2)$.*

Proof. The operator is densely defined in $L^2(\mathscr{S}_\omega;\mathbb{C}^2)$, because $C_0^\infty(\mathscr{S}_\omega;\mathbb{C}^2)\subset \operatorname{dom}\mathsf{D}_\omega$ is dense in $L^2(\mathscr{S}_\omega;\mathbb{C}^2)$. Since $\mathscr{S}_\omega$ is the epigraph of a globally Lipschitz function, it is straightforward to derive from [13, Thm. 3.34 and 3.38] that the Green's identity

$$\int_{\mathscr{S}_\omega}(-\mathrm{i}\sigma\cdot\nabla)u\cdot\overline{v}\,\mathrm{d}x-\int_{\mathscr{S}_\omega}u\cdot\overline{(-\mathrm{i}\sigma\cdot\nabla)v}\,\mathrm{d}x=-\mathrm{i}\int_{\Gamma_\omega^+\cup\Gamma_\omega^-}((\sigma\cdot\mathbf{n})u)\cdot\overline{v}\,\mathrm{d}s$$

holds for all $u,v\in H^1(\mathscr{S}_\omega;\mathbb{C}^2)$; *cf.* [18, Lem. 1.4 (i)] for the same formula on bounded piecewise-C^1 domains. Hence, for any $u,v\in\operatorname{dom}\mathsf{D}_\omega$ we have that

$$(\mathsf{D}_\omega u,v)_{\mathscr{S}_\omega}-(u,\mathsf{D}_\omega v)_{\mathscr{S}_\omega}=-\mathrm{i}\int_{\Gamma_\omega^+\cup\Gamma_\omega^-}((\sigma\cdot\mathbf{n})u)\cdot\overline{v}\,\mathrm{d}s \tag{2.1}$$

Thanks to the boundary conditions (1.3), we have that

$$\begin{aligned}\int_{\Gamma_\omega^+\cup\Gamma_\omega^-}((\sigma\cdot\mathbf{n})u)\cdot\overline{v}\,\mathrm{d}s&=\int_{\Gamma_\omega^+}(\sigma\cdot\mathbf{n})(-\mathrm{i}\sigma_3(\sigma\cdot\mathbf{n}))u\cdot\overline{(-\mathrm{i}\sigma_3(\sigma\cdot\mathbf{n}))v}\,\mathrm{d}s\\&\quad+\int_{\Gamma_\omega^-}(\sigma\cdot\mathbf{n})(\mathrm{i}\sigma_3(\sigma\cdot\mathbf{n}))u\cdot\overline{(\mathrm{i}\sigma_3(\sigma\cdot\mathbf{n}))v}\,\mathrm{d}s.\end{aligned}$$

Since $\pm\mathrm{i}\sigma_3(\sigma\cdot\mathbf{n})$ are symmetric $\mathbb{C}^{2\times2}$ matrices, we have that

$$\begin{aligned}\int_{\Gamma_\omega^+\cup\Gamma_\omega^-}((\sigma\cdot\mathbf{n})u)\cdot\overline{v}\,\mathrm{d}s&=-\int_{\Gamma_\omega^+\cup\Gamma_\omega^-}\sigma_3(\sigma\cdot\mathbf{n})(\sigma\cdot\mathbf{n})\sigma_3(\sigma\cdot\mathbf{n})u\cdot\overline{v}\,\mathrm{d}s\\&=-\int_{\Gamma_\omega^+\cup\Gamma_\omega^-}((\sigma\cdot\mathbf{n})u)\cdot\overline{v}\,\mathrm{d}s,\end{aligned}$$

where in the last equality we have used the fact that $(\sigma\cdot\mathbf{n})^2=\sigma_3^2=\mathbb{I}_2$. We conclude that the right hand side in (2.1) vanishes, and consequently that D_ω is symmetric.

2.2. Representation in polar coordinates

Let us introduce polar coordinates (r,θ) on $\mathscr{S}_\omega$. They are related to the Cartesian coordinates $x=(x_1,x_2)$ *via* the identities

$$x(r,\theta)=\begin{pmatrix}x_1(r,\theta)\\x_2(r,\theta)\end{pmatrix},\quad\text{where}\quad x_1=x_1(r,\theta)=r\cos\theta,\quad x_2=x_2(r,\theta)=r\sin\theta,$$

for all $r > 0$ and $\theta \in \mathbb{I}_\omega = (-\omega, \omega)$. Further, we consider the moving frame $(\mathbf{e}_{\mathrm{rad}}, \mathbf{e}_{\mathrm{ang}})$ associated with the polar coordinates

$$\mathbf{e}_{\mathrm{rad}}(\theta) = \frac{\mathrm{d}x}{\mathrm{d}r} = \begin{pmatrix} \cos\theta \\ \sin\theta \end{pmatrix} \quad \text{and} \quad \mathbf{e}_{\mathrm{ang}}(\theta) = \frac{\mathrm{d}\mathbf{e}_{\mathrm{rad}}}{\mathrm{d}\theta} = \begin{pmatrix} -\sin\theta \\ \cos\theta \end{pmatrix}.$$

The Hilbert space $L^2_{\mathrm{cyl}}(\mathscr{S}_\omega;\mathbb{C}^2) := L^2(\mathbb{R}_+ \times \mathbb{I}_\omega, \mathbb{C}^2; r\mathrm{d}r\mathrm{d}\theta)$ can be viewed as the tensor product $L^2_r(\mathbb{R}_+) \otimes L^2(\mathbb{I}_\omega;\mathbb{C}^2)$, where the weighted L^2-space $L^2_r(\mathbb{R}_+)$ is defined as

$$L^2_r(\mathbb{R}_+) = \left\{ \psi \colon \mathbb{R}_+ \to \mathbb{C} \colon \int_{\mathbb{R}_+} |\psi|^2 r\mathrm{d}r < \infty \right\}.$$

Let us consider the unitary transform

$$\mathsf{V} \colon L^2(\mathscr{S}_\omega;\mathbb{C}^2) \to L^2_{\mathrm{cyl}}(\mathscr{S}_\omega;\mathbb{C}^2), \qquad (\mathsf{V}v)(r,\theta) = u\big(r\cos\theta, r\sin\theta\big),$$

and introduce the cylindrical Sobolev space by

$$H^1_{\mathrm{cyl}}(\mathscr{S}_\omega;\mathbb{C}^2) := \mathsf{V}\big(H^1(\mathscr{S}_\omega;\mathbb{C}^2)\big) = \left\{ v \colon v, \partial_r v, r^{-1}(\partial_\theta v) \in L^2_{\mathrm{cyl}}(\mathscr{S}_\omega;\mathbb{C}^2) \right\}.$$

We consider the operator acting in the Hilbert space $L^2_{\mathrm{cyl}}(\mathscr{S}_\omega;\mathbb{C}^2)$ and defined as

$$\widetilde{\mathsf{D}}_\omega := \mathsf{V}\mathsf{D}_\omega\mathsf{V}^{-1}, \qquad \mathrm{dom}\,\widetilde{\mathsf{D}}_\omega := \mathsf{V}\big(\mathrm{dom}\,\mathsf{D}_\omega\big). \tag{2.2}$$

Now, let us compute the action of $\widetilde{\mathsf{D}}_\omega$ on a function $v \in \mathrm{dom}\,\widetilde{\mathsf{D}}_\omega$. First, notice that there exists a unique $u \in \mathrm{dom}\,\mathsf{D}_\omega$ such that $v = \mathsf{V}u$ and the partial derivatives of u with respect to the Cartesian variables (x_1, x_2) can be expressed through those of v with respect to polar variables (r,θ) via the standard relations (for $x = x(r,\theta)$)

$$\begin{aligned} (\partial_1 u)(x) &= \cos\theta(\partial_r v)(r,\theta) - \sin\theta\frac{(\partial_\theta v)(r,\theta)}{r}, \\ (\partial_2 u)(x) &= \sin\theta(\partial_r v)(r,\theta) + \cos\theta\frac{(\partial_\theta v)(r,\theta)}{r}. \end{aligned}$$

Using the latter formulæ we can express the action of the differential expression $\mathscr{D} = -\mathrm{i}(\sigma\cdot\nabla)$ in polar coordinates as follows (for $x = x(r,\theta)$)

$$(\mathscr{D}u)(x) = -\mathrm{i}\begin{pmatrix} \partial_1 u_2(x) - \mathrm{i}\partial_2 u_2(x) \\ \partial_1 u_1(x) + \mathrm{i}\partial_2 u_1(x) \end{pmatrix} = -\mathrm{i}\begin{pmatrix} e^{-\mathrm{i}\theta}(\partial_r v_2)(r,\theta) - \mathrm{i}e^{-\mathrm{i}\theta}r^{-1}(\partial_\theta v_2)(r,\theta) \\ e^{\mathrm{i}\theta}(\partial_r v_1)(r,\theta) + \mathrm{i}e^{\mathrm{i}\theta}r^{-1}(\partial_\theta v_1)(r,\theta) \end{pmatrix}.$$

Note that a basic computation yields

$$\sigma\cdot\mathbf{e}_{\mathrm{rad}} = \cos\theta\sigma_1 + \sin\theta\sigma_2 = \begin{pmatrix} 0 & e^{-\mathrm{i}\theta} \\ e^{\mathrm{i}\theta} & 0 \end{pmatrix}. \tag{2.3}$$

Hence, the operator $\widetilde{\mathsf{D}}_\omega$ acts as

$$\begin{aligned} \widetilde{\mathsf{D}}_\omega v &= -\mathrm{i}(\sigma\cdot\mathbf{e}_{\mathrm{rad}})\left(\partial_r v + \frac{v}{2r} - \frac{(-\mathrm{i}\sigma_3\partial_\theta + \frac{1}{2})v}{r}\right), \\ \mathrm{dom}\,\widetilde{\mathsf{D}}_\omega &= \big\{ v \in H^1_{\mathrm{cyl}}(\mathscr{S}_\omega;\mathbb{C}^2) \colon v_2(\cdot,\pm\omega) = -e^{\pm\mathrm{i}\omega}v_1(\cdot,\pm\omega) \big\}. \end{aligned} \tag{2.4}$$

3. Orthogonal decomposition

Now, we introduce an auxiliary spin-orbit-type operator in the Hilbert space $(L^2(\mathbb{I}_\omega;\mathbb{C}^2),(\cdot,\cdot)_{\mathbb{I}_\omega})$ as follows

$$\begin{aligned} \mathsf{J}_\omega\phi &= -\mathrm{i}\sigma_3\phi' + \frac{\phi}{2} = \begin{pmatrix} -\mathrm{i}\phi_1' + \frac{\phi_1}{2} \\ +\mathrm{i}\phi_2' + \frac{\phi_2}{2} \end{pmatrix}, \\ \operatorname{dom}\mathsf{J}_\omega &= \Big\{\phi = (\phi_1,\phi_2) \in H^1(\mathbb{I}_\omega;\mathbb{C}^2)\colon \phi_2(\pm\omega) = -e^{\pm\mathrm{i}\omega}\phi_1(\pm\omega)\Big\}. \end{aligned} \tag{3.1}$$

Let us investigate the spectral properties of J_ω.

PROPOSITION 3.1. *Let the operator J_ω be as in (3.1). Then the following hold:*

(i) J_ω *is self-adjoint and has a compact resolvent.*

(ii) $\sigma(\mathsf{J}_\omega) = \{\lambda_k\}_{k\in\mathbb{Z}} = \left\{\frac{\pi k}{2\omega}\right\}_{k\in\mathbb{Z}}$ *and* $\mathscr{F}_k := \ker\left(\mathsf{J}_\omega - \lambda_k\right) = \mathsf{span}\{\phi_k\}$, *where*

$$\phi_k(\theta) = \frac{1}{2\sqrt{\omega}}\begin{pmatrix} e^{+\mathrm{i}(\lambda_k-\frac{1}{2})\theta} \\ (-1)^{k+1}e^{-\mathrm{i}(\lambda_k-\frac{1}{2})\theta} \end{pmatrix}; \tag{3.2}$$

moreover, $\{\phi_k\}_{k\in\mathbb{Z}}$ *is an orthonormal basis of* $L^2(\mathbb{I}_\omega;\mathbb{C}^2)$.

(iii) $(\sigma\cdot\mathbf{e}_{\mathrm{rad}})\phi_k = (-1)^{k+1}\phi_{-k}$ *for all* $k\in\mathbb{Z}$.

Proof. (i) The operator $\mathsf{J}_\omega - \frac{1}{2}$ can be viewed as a momentum operator on a graph with two edges of length 2ω, in which the vectors $\phi^{\mathrm{out}} := \{\phi_1(-\omega),\phi_2(\omega)\}$ and $\phi^{\mathrm{in}} := \{\phi_1(\omega),\phi_2(-\omega)\}$ are connected as $\phi^{\mathrm{out}} = U\phi^{\mathrm{in}}$ via the unitary matrix

$$U = \begin{pmatrix} 0 & -e^{\mathrm{i}\omega} \\ -e^{\mathrm{i}\omega} & 0 \end{pmatrix}.$$

Hence, $\mathsf{J}_\omega - \frac{1}{2}$ is self-adjoint by [8, Prop. 4.1] and has a compact resolvent by [8, Thm. 5.1]. Adding a constant $\frac{1}{2}$ has no impact on these properties and hence the claim follows.

(ii) Let $\phi = (\phi_1,\phi_2)^\top \in \operatorname{dom}\mathsf{J}_\omega$ and $\lambda\in\mathbb{R}$ be such that $\mathsf{J}_\omega\phi = \lambda\phi$. The eigenvalue equation on ϕ reads as follows

$$\begin{aligned} -\mathrm{i}\phi_1' + \frac{\phi_1}{2} &= \lambda\phi_1, \\ +\mathrm{i}\phi_2' + \frac{\phi_2}{2} &= \lambda\phi_2. \end{aligned}$$

The generic solution of the above system of differential equations is given by

$$\begin{cases} \phi_1(\theta) = a_1 e^{+\mathrm{i}(\lambda-\frac{1}{2})\theta}, \\ \phi_2(\theta) = a_2 e^{-\mathrm{i}(\lambda-\frac{1}{2})\theta}, \end{cases} \qquad a_1,a_2\in\mathbb{C}.$$

Hence, the boundary conditions yield

$$\begin{cases} a_1 e^{+\mathrm{i}\omega} e^{+\mathrm{i}(\lambda-\frac{1}{2})\omega} + a_2 e^{-\mathrm{i}(\lambda-\frac{1}{2})\omega} = 0, \\ a_1 e^{-\mathrm{i}\omega} e^{-\mathrm{i}(\lambda-\frac{1}{2})\omega} + a_2 e^{+\mathrm{i}(\lambda-\frac{1}{2})\omega} = 0, \end{cases}$$

that can be simplified as

$$\begin{cases} a_1 e^{+\mathrm{i}(\lambda+\frac{1}{2})\omega} + a_2 e^{-\mathrm{i}(\lambda-\frac{1}{2})\omega} = 0, \\ a_1 e^{-\mathrm{i}(\lambda+\frac{1}{2})\omega} + a_2 e^{+\mathrm{i}(\lambda-\frac{1}{2})\omega} = 0. \end{cases}$$

This system has a non-trivial solution if the corresponding determinant vanishes, that is

$$\Delta = e^{+\mathrm{i}(\lambda+\frac{1}{2})\omega} e^{+\mathrm{i}(\lambda-\frac{1}{2})\omega} - e^{-\mathrm{i}(\lambda-\frac{1}{2})\omega} e^{-\mathrm{i}(\lambda+\frac{1}{2})\omega} = e^{+2\mathrm{i}\lambda\omega} - e^{-2\mathrm{i}\lambda\omega} = 2\mathrm{i}\sin(2\lambda\omega),$$

and consequently the eigenvalues are given by

$$\lambda_k = \frac{\pi k}{2\omega}, \qquad k \in \mathbb{Z}.$$

The corresponding eigenvectors can be recovered with the aid of the formula

$$a_1 e^{+\mathrm{i}\left(\frac{\pi k}{2}+\frac{\omega}{2}\right)} + a_2 e^{-\mathrm{i}\left(\frac{\pi k}{2}-\frac{\omega}{2}\right)} = 0$$

which leads to $a_1 e^{\mathrm{i}\pi k} + a_2 = 0$. The choice

$$a_1 = \frac{1}{2\sqrt{\omega}}, \qquad a_2 = \frac{(-1)^{k+1}}{2\sqrt{\omega}}$$

yields the orthonormal basis in (3.2).

(iii) Using (2.3) we obtain

$$\begin{aligned} (\sigma\cdot\mathbf{e}_{\mathrm{rad}})\phi_k &= \frac{1}{2\sqrt{\omega}} \begin{pmatrix} 0 & e^{-\mathrm{i}\theta} \\ e^{\mathrm{i}\theta} & 0 \end{pmatrix} \begin{pmatrix} e^{+\mathrm{i}(\lambda_k-\frac{1}{2})\theta} \\ (-1)^{k+1} e^{-\mathrm{i}(\lambda_k-\frac{1}{2})\theta} \end{pmatrix} \\ &= \frac{1}{2\sqrt{\omega}} \begin{pmatrix} (-1)^{k+1} e^{-\mathrm{i}(\lambda_k+\frac{1}{2})\theta} \\ e^{\mathrm{i}(\lambda_k+\frac{1}{2})\theta} \end{pmatrix} \\ &= \frac{1}{2\sqrt{\omega}} (-1)^{k+1} \begin{pmatrix} e^{\mathrm{i}(\lambda_{-k}-\frac{1}{2})\theta} \\ (-1)^{k+1} e^{-\mathrm{i}(\lambda_{-k}-\frac{1}{2})\theta} \end{pmatrix} = (-1)^{k+1}\phi_{-k}. \quad \square \end{aligned}$$

Further, we employ the orthogonal decomposition

$$L^2_{\mathrm{cyl}}(\mathscr{S}_\omega;\mathbb{C}^2) \simeq L^2_r(\mathbb{R}_+) \otimes L^2(\mathbb{I}_\omega;\mathbb{C}^2) = \oplus_{k\in\mathbb{N}_0}\mathscr{E}_k,$$

where $\mathscr{E}_0 = L^2_r(\mathbb{R}) \otimes \mathscr{F}_0$ and $\mathscr{E}_k = L^2_r(\mathbb{R}) \otimes (\mathscr{F}_k \oplus \mathscr{F}_{-k})$ for $k \in \mathbb{N}$. In the following proposition we show that $\mathscr{E}_k$ are reducing subspaces for $\widetilde{\mathsf{D}}_\omega$. The analysis of $\widetilde{\mathsf{D}}_\omega$ boils down to the study of its restrictions to these subspaces. For the sake of convenience, we introduce the unitary transforms $\mathsf{W}_0\colon \mathscr{E}_0 \to L^2(\mathbb{R}_+)$ and $\mathsf{W}_k\colon \mathscr{E}_k \to L^2(\mathbb{R}_+;\mathbb{C}^2)$ for $k \in \mathbb{N}$ as

$$(\mathsf{W}_0 u)(r) := \sqrt{r}\,\big(u(r,\cdot),\phi_0\big)_{\mathbb{I}_\omega}, \quad (\mathsf{W}_k u)(r) := \sqrt{r}\begin{pmatrix} (u(r,\cdot),\phi_k)_{\mathbb{I}_\omega} \\ \mathrm{i}(u(r,\cdot),\phi_{-k})_{\mathbb{I}_\omega} \end{pmatrix}.$$

PROPOSITION 3.2. *For any $k \in \mathbb{N}_0$,*

$$d_k u := \widetilde{\mathsf{D}}_\omega u, \qquad \operatorname{dom} d_k := \operatorname{dom}\widetilde{\mathsf{D}}_\omega \cap \mathscr{E}_k,$$

is a well-defined operator in the Hilbert space $\mathscr{E}_k$.

The operator d_0 is unitarily equivalent via W_0 to the operator $\mathbf{d}_0$ in the Hilbert space $L^2(\mathbb{R}_+)$ defined as

$$\mathbf{d}_0\psi := \mathrm{i}\psi', \qquad \operatorname{dom}\mathbf{d}_0 := H^1_0(\mathbb{R}_+). \tag{3.3}$$

For any $k \in \mathbb{N}$, the operator d_k is unitarily equivalent via W_k to the operator $\mathbf{d}_k$ in the Hilbert space $L^2(\mathbb{R}_+)$ defined as

$$\mathbf{d}_k := (-1)^{k+1}\begin{pmatrix} 0 & -\frac{\mathsf{d}}{\mathsf{d}r} - \frac{\pi k}{2\omega r} \\ \frac{\mathsf{d}}{\mathsf{d}r} - \frac{\pi k}{2\omega r} & 0 \end{pmatrix}, \qquad \operatorname{dom}\mathbf{d}_k := H^1_0(\mathbb{R}_+;\mathbb{C}^2). \tag{3.4}$$

In particular, the decomposition

$$\mathsf{D}_\omega \simeq \bigoplus_{k\in\mathbb{N}_0} \mathbf{d}_k$$

holds and the deficiency indices of D_ω can be computed as $n_\pm(\mathsf{D}_\omega) = \sum_{k\in\mathbb{N}_0} n_\pm(\mathbf{d}_k)$.

Proof. *Step 1: $k=0$.* Pick a function $u \in \operatorname{dom}\widetilde{\mathsf{D}}_\omega \cap \mathscr{E}_0$. By definition, u writes as

$$u(r,\theta) = \frac{\psi_0(r)}{\sqrt{r}}\phi_0(\theta),$$

with some $\psi_0\colon \mathbb{R}_+ \to \mathbb{C}$. Next, we observe that $u \in H^1_{\mathrm{cyl}}(\mathscr{S}_\omega;\mathbb{C}^2)$ is equivalent to $u, \partial_r u, \frac{\partial_\theta u}{r} \in L^2_r(\mathbb{R}_+)$, which is, in its turn, equivalent to $\psi_0, \left(\frac{\psi_0}{\sqrt{r}}\right)'\sqrt{r}, \frac{\psi_0}{r} \in L^2(\mathbb{R}_+)$. Now, we aim at showing the following equivalence

$$u \in H^1_{\mathrm{cyl}}(\mathscr{S}_\omega;\mathbb{C}^2) \quad\Longleftrightarrow\quad \psi_0 \in H^1_0(\mathbb{R}_+). \tag{3.5}$$

First, we obtain that

$$\psi_0' = \left(\frac{\psi_0}{\sqrt{r}}\right)'\sqrt{r} + \frac{1}{2}\frac{\psi_0}{r} \in L^2(\mathbb{R}_+).$$

Hence, $u \in H^1_{\mathrm{cyl}}(\mathscr{S}_\omega;\mathbb{C}^2)$ implies $\psi_0 \in H^1(\mathbb{R}_+)$. Moreover, thanks e.g. to [6, Prop. 2.2 (i)] (with $a=0$ settled there) we infer that there exists $\mathsf{p} \in \mathbb{C}$ such that

$$\lim_{r\to 0^+} |\psi_0(r) - \mathsf{p}|r^{-1/2} = 0,$$

and, according to [6, Prop. 2.4 (i)] (for $a=0$), we obtain that $\frac{\psi_0-\mathsf{p}}{r}\in L^2(\mathbb{R}_+)$. Since $\frac{\psi_0}{r}\in L^2(\mathbb{R}_+)$, we get that $\mathsf{p}=0$. Hence, by the Sobolev trace theorem we obtain that $\psi_0\in H_0^1(\mathbb{R}_+)$. The reverse implication in (3.5) immediately follows from the one-dimensional Hardy inequality; see e.g. [6, Prop. 2.4 (i)].

Applying the differential expression obtained in (2.4) to u, we get

$$(\widetilde{\mathsf{D}}_\omega u)(r,\theta)=-\mathsf{i}(\sigma\cdot\mathbf{e}_{\mathrm{rad}})\phi_0(\theta)\left(\partial_r\left(\frac{\psi_0(r)}{\sqrt{r}}\right)+\frac{\psi_0(r)}{2r^{3/2}}\right)=\mathsf{i}\frac{\psi_0'(r)}{\sqrt{r}}\phi_0(\theta). \tag{3.6}$$

Step 2: $k\in\mathbb{N}$. Pick a function $u\in\operatorname{dom}\widetilde{\mathsf{D}}_\omega\cap\mathscr{E}_k$. By definition, u writes as

$$u(r,\theta)=\frac{\psi_{+k}(r)}{\sqrt{r}}\phi_k(\theta)-\mathsf{i}\frac{\psi_{-k}(r)}{\sqrt{r}}\phi_{-k}(\theta),$$

with some $\psi_{\pm k}\colon\mathbb{R}_+\to\mathbb{C}$. Observe that

$$\begin{aligned}(\phi_k',\phi_{-k}')_{\mathbb{I}_\omega}&=-((\mathsf{i}\sigma_3)^2\phi_k',\phi_{-k}')_{\mathbb{I}_\omega}=(-\mathsf{i}\sigma_3\phi_k',-\mathsf{i}\sigma_3\phi_{-k}')_{\mathbb{I}_\omega}\\&=\left(\lambda_k-\frac12\right)\left(\lambda_{-k}-\frac12\right)(\phi_k,\phi_{-k})_{\mathbb{I}_\omega}=0.\end{aligned} \tag{3.7}$$

Again, $u\in H^1_{\mathrm{cyl}}(\mathscr{S}_\omega;\mathbb{C}^2)$ is equivalent to $u,\partial_r u,\frac{\partial_\theta u}{r}\in L^2_r(\mathbb{R}_+)$. Taking into account orthogonality (3.7), $u\in H^1_{\mathrm{cyl}}(\mathscr{S}_\omega;\mathbb{C}^2)$ is equivalent to $\psi_{\pm k},\left(\frac{\psi_{\pm k}}{\sqrt{r}}\right)'\sqrt{r},\frac{\psi_{\pm k}}{r}\in L^2(\mathbb{R}_+)$ and as in the case $k=0$ we end up with equivalence between $u\in H^1_{\mathrm{cyl}}(\mathscr{S}_\omega;\mathbb{C}^2)$ and $\psi_{\pm k}\in H^1_0(\mathbb{R}_+)$. Applying the differential expression obtained in (2.4), we get

$$\begin{aligned}\widetilde{\mathsf{D}}_\omega u&=-\frac{\mathsf{i}(\sigma\cdot\mathbf{e}_{\mathrm{rad}})}{\sqrt{r}}\left[\phi_k\left(\partial_r\psi_k-\frac{\lambda_k\psi_k}{r}\right)-\mathsf{i}\phi_{-k}\left(\partial_r\psi_{-k}-\frac{\lambda_{-k}\psi_{-k}}{r}\right)\right]\\&=\frac{(-1)^{k+1}}{\sqrt{r}}\left[-\mathsf{i}\phi_{-k}\left(\partial_r\psi_k-\frac{\lambda_k\psi_k}{r}\right)+\phi_k\left(-\partial_r\psi_{-k}-\frac{\lambda_k\psi_{-k}}{r}\right)\right].\end{aligned} \tag{3.8}$$

Step 3: Conclusion of the proof. The analysis in Steps 1 and 2 yields that the inclusion $\widetilde{\mathsf{D}}_\omega\left(\operatorname{dom}\widetilde{\mathsf{D}}_\omega\cap\mathscr{E}_k\right)\subset\mathscr{E}_k$ holds for all $k\in\mathbb{N}_0$. Hence, the operators d_k are symmetric for all $k\in\mathbb{N}_0$. Relying on formulae (3.6) and (3.8) we find that

$$\mathsf{W}_k d_k\mathsf{W}_k^{-1}=\mathbf{d}_k,\qquad\forall k\in\mathbb{N}_0.\quad\square$$

4. Proofs of the main results

With all the preparations above the proofs of the main results are rather compact.

Proof of Theorem 1.1. For all $k\in\mathbb{N}$ the operators $\mathbf{d}_k$ are self-adjoint thanks to [6, Thm. 1.1 (i) and Prop. 3.1 (i)], since for all $k\in\mathbb{N}$ we have $\gamma:=\left|\frac{k\pi}{2\omega}\right|>\frac12$.

By a direct computation it is elementary to observe that

$$\mathbf{d}_0^*=\mathsf{i}\psi',\qquad\operatorname{dom}\mathbf{d}_0^*=H^1(\mathbb{R}_+).$$

Hence,

$$\ker(\mathbf{d}_0^* - \mathsf{i}) = \{0\} \quad \text{and} \quad \ker(\mathbf{d}_0^* + \mathsf{i}) = \mathsf{span}\,\{e^{-r}\}.$$

The deficiency indices of $\mathbf{d}_0$ are given by $(0,1)$ and the corresponding defect element is $\psi_\star(r) = e^{-r}$. Hence, by Proposition 3.2 the operators $\widetilde{\mathsf{D}}_\omega$ and D_ω have deficiency indices $(0,1)$ as well and the defect element of D_ω is given in polar coordinates by

$$u_\star(r,\theta) = \left(\mathsf{W}_0^{-1}\psi_\star\right)(r,\theta) = \frac{e^{-r}}{\sqrt{r}}\phi_0(\theta) = \frac{1}{2\sqrt{\varpi}}\frac{e^{-r}}{\sqrt{r}}\begin{pmatrix} e^{-\frac{\mathsf{i}\theta}{2}} \\ -e^{\frac{\mathsf{i}\theta}{2}} \end{pmatrix}. \quad \square$$

Proof of Theorem 1.2. Since the operator D_ω has deficiency indices $(0,1)$, the operator $-\mathsf{D}_\omega$ has deficiency indices $(1,0)$, respectively, and moreover $\ker(\mathsf{D}_\omega^* + \mathsf{i}) = \ker((-\mathsf{D}_\omega)^* - \mathsf{i}) = \mathsf{span}\,\{u_\star\}$. Therefore, the deficiency indices of the operator $\mathsf{M}_\omega = \mathsf{D}_\omega \oplus (-\mathsf{D}_\omega)$ are $(1,1)$ and its defect subspaces are given by

$$\ker(\mathsf{M}_\omega^* - \mathsf{i}) = \mathsf{span}\left\{\begin{pmatrix} 0 \\ u_\star \end{pmatrix}\right\} \qquad \text{and} \qquad \ker(\mathsf{M}_\omega^* + \mathsf{i}) = \mathsf{span}\left\{\begin{pmatrix} u_\star \\ 0 \end{pmatrix}\right\}.$$

Hence, by [19, Thm. X.2] all the self-adjoint extensions of M_ω are parametrized by $\alpha \in \mathbb{T}$ as follows

$$\mathsf{M}_{\alpha,\omega} := \begin{pmatrix} \mathscr{D}u_1 + \mathsf{i}u_\star \\ -\mathscr{D}u_2 - \mathsf{i}\alpha u_\star \end{pmatrix}, \quad \operatorname{dom}\mathsf{M}_{\alpha,\omega} := \left\{\begin{pmatrix} u_1 \\ u_2 \end{pmatrix} + \begin{pmatrix} u_\star \\ \alpha u_\star \end{pmatrix} : u_1, u_2 \in \operatorname{dom}\mathsf{D}_\omega\right\},$$

by which the proof is concluded. $\square$

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(Received August 7, 2020)

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