

# SPECTRA OF GRAPHENES WITH VARIANT EDGES

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**Abstract.** In this paper, we consider a periodic quantum graph corresponding to graphene with a variant of the zigzag shape of boundaries. The aim of this paper is to compare the spectra of our graphs with the spectra of quantum graphs with the standard zigzag boundaries. For this purpose, we utilize a Shnol type theorem and the Cramer's rule to construct two spectral discriminants  $D_s(\mu, \lambda)$  and  $D_c(\mu, \lambda)$ , where  $\mu = S^1 := [-\pi, \pi)$  is a quasi-momentum of a corresponding fiber operator and  $\lambda \in \mathbb{R}$  is a spectral parameter. As a result, we derive pictures of a part of the dispersion relation for our quantum graph.

## 1. Introduction and main results

From a point of view of topological insulators, it is important to compare the spectral structure of the system in a whole space with the spectral structure of the system in a half space with boundaries. Indeed, topological insulators are known as materials that behave as insulators in its bulk (interior) but contain conducting states (edge states) in their surface (edge). Let  $k \in S^1 := [-\pi, \pi)$  be a quasi-momentum. In order to construct a  $\mathbb{Z}_2$ -invariant between bulk and edge Hamiltonians, Graf and Porta [3] dealt with the  $k$ -parametrized bulk Hamiltonian  $H_{\text{GP}}(k)$  in  $\ell^2(\mathbb{Z}; \mathbb{C}^N)$  and the  $k$ -parametrized edge Hamiltonian  $H_{\text{GP}}^\sharp(k)$  in  $\ell^2(\mathbb{N}; \mathbb{C}^N)$  acting as

$$\begin{aligned} (H_{\text{GP}}(k)\psi)_n &= A(k)\psi_{n-1} + A(k)^*\psi_{n+1} + V_n(k)\psi_n, & n \in \mathbb{Z}, & \quad \psi = (\psi_n)_{n \in \mathbb{Z}}, \\ (H_{\text{GP}}^\sharp(k)\psi)_n &= A(k)\psi_{n-1} + A(k)^*\psi_{n+1} + V_n^\sharp(k)\psi_n, & n \in \mathbb{N}, & \quad \psi = (\psi_n)_{n \in \mathbb{N}}. \end{aligned}$$

Here, the potential  $V_n(k), V_n^\sharp(k)$  and the hopping matrices  $A(k)$  are  $N \times N$  matrices satisfying suitable assumptions (see [3]). Since the operators  $H_{\text{GP}}(k)$  and  $H_{\text{GP}}^\sharp(k)$  play role of the fiber operators of the discrete Schrödinger operators in Graphene or the Kane–Male model [4] of topological insulators under the suitable choices of  $A(k)$  and potentials in the case of  $N = 2$ ,  $H_{\text{GP}}(k)$  and  $H_{\text{GP}}^\sharp(k)$  are considered as a generalization of a class of fiber operators.

In this paper, we study the spectra of the periodic Hamiltonian  $H^b$  on Graphene with variant boundaries (see Fig. 1) from the point of view of the quantum graphs. The aim of this paper is to compare the spectrum of our Hamiltonian  $H^b$  with the spectrum

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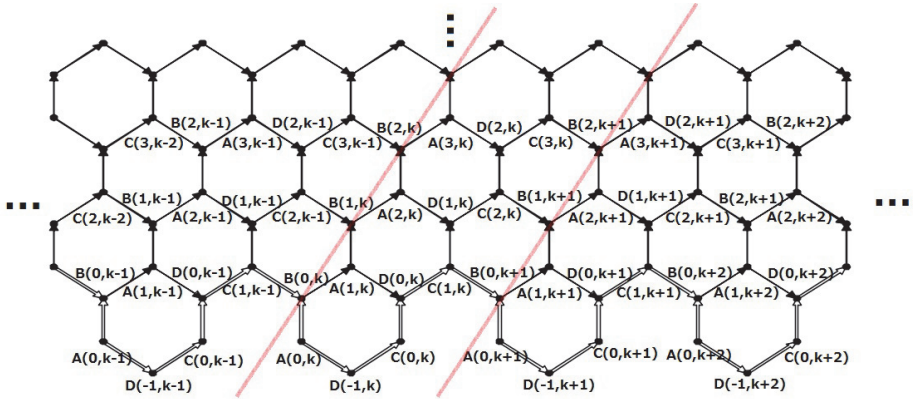


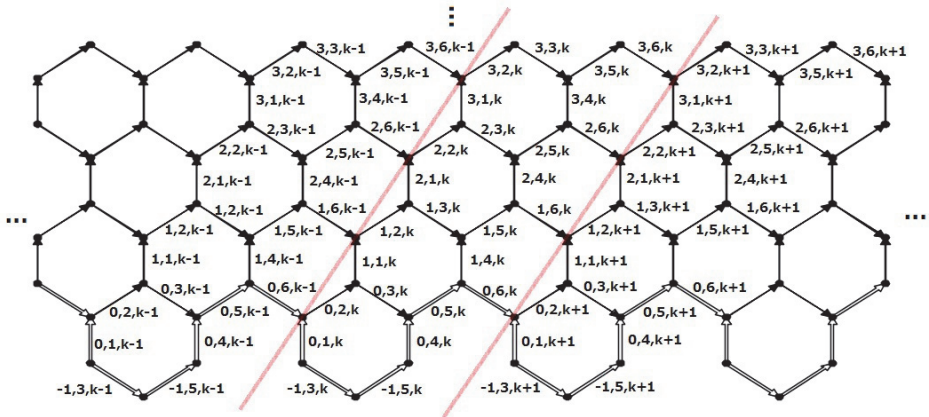
Fig. 1: The metric graph  $\Gamma^b$  for the edge Hamiltonian  $H^b$  with the variant boundaries. The points  $A_{n,k}, B_{n,k}, C_{n,k}, D_{n,k}$  are denoted by  $A(n,k), B(n,k), C(n,k), D(n,k)$ .

of the periodic edge Hamiltonian  $H^\sharp$  in [8] on the Graphene with the standard zigzag boundaries. Let us state the definition of the main target Hamiltonian  $H^b$ . At first, we recall that a quantum graph is defined as a triple of a metric graph, a differential Schrödinger operator, and a suitable vertex condition [1]. We define the metric graph  $\Gamma^b$  as the hexagonal lattice with the variant shape of boundaries as seen in Fig. 1. Let  $E^b$  and  $V^b$  be the set of edges and vertices of  $\Gamma^b$ , respectively:  $\Gamma^b = \{E^b, V^b\}$ . For an edge  $e \in E^b$ , its orientation is given as seen in Fig. 1. A white (black, respectively) arrow is located on the boundary (in the interior, respectively) of  $\Gamma^b$ . The set of vertices  $V^b$  consists of the points  $A_{n,k}, B_{n,k}, C_{n,k}, D_{n,k}$  ( $n = 0, 1, 2, \dots$ ) and  $D_{-1,k}$ , where  $k \in \mathbb{Z}$ . Put  $\mathcal{J} = \{1, 2, 3, 4, 5, 6\}$  and  $\mathcal{Z} = \mathcal{Z}_1 \cup \mathcal{Z}_2 \cup \mathcal{Z}_3$ , where  $\mathcal{Z}_1 = \mathbb{N} \times \mathcal{J} \times \mathbb{Z}$ ,  $\mathcal{Z}_2 = \{0\} \times \{2, 3\} \times \mathbb{Z}$ ,  $\mathcal{Z}_3 = \{(0, 1), (0, 4), (0, 5), (0, 6), (-1, 3), (-1, 5)\} \times \mathbb{Z}$ . For distinct points  $A$  and  $B$  in  $\mathbb{R}^2$ , we denote the segments connecting  $A$  and  $B$  by  $AB$  and  $\overline{AB}$ , where  $AB$  does not contain the edges  $A$  and  $B$  although  $\overline{AB}$  does contain  $A$  and  $B$ . In order to identify which edge is under consideration, we give an address  $(n, j, k) \in \mathbb{Z}$  for an edge  $e \in E^b$  to derive the one-to-one correspondence between  $\mathcal{Z}$  and  $E^b$  such as  $E^b = \{e_{n,j,k} \mid (n, j, k) \in \mathcal{Z}\}$  (see also Fig. 2), where

$$\begin{aligned} e_{n,1,k} &= A_{n,k}B_{n,k}, & e_{n,2,k} &= B_{n,k}A_{n+1,k}, & e_{n,3,k} &= A_{n+1,k}D_{n,k}, \\ e_{n,4,k} &= C_{n,k}D_{n,k}, & e_{n,5,k} &= D_{n,k}C_{n+1,k}, & e_{n,6,k} &= C_{n+1,k}B_{n,k+1}. \end{aligned}$$

We assume that the length of any edge  $e \in E^b$  is 1. For any  $(n, j, k) \in \mathcal{Z}$ , we give the identification  $e_{n,j,k} \simeq (0, 1)$ , where  $x = 0$  and  $x = 1$  corresponds to the initial and terminal vertices of  $e_{n,j,k}$ . For a function  $y$  on  $\Gamma^b$ , we denote  $y$  restricted on  $e_{n,j,k}$  by  $y_{n,j,k}$ . Fix a real-valued potential  $q \in L^2(0, 1)$  and suppose that

$$\operatorname{ess\,inf}_{x \in (0,1)} q(x) > -\infty$$

Fig. 2: The metric graph  $\Gamma^b$ .

throughout this paper. In this paper, we study the Schrödinger operator

$$(H^b y)_{n,j,k}(x) = -y''_{n,j,k}(x) + q(x)y_{n,j,k}(x), \quad x \in (0,1) \simeq e_{n,j,k}, \quad (n,j,k) \in \mathcal{Z}$$

in the Hilbert space  $L^2(\Gamma^b) = \bigoplus_{(n,j,k) \in \mathcal{Z}} L^2(e_{n,j,k})$ , where  $L^2(e_{n,j,k}) = L^2(0,1)$ . Let  $y \in \text{dom}(H^b)$  be imposed the Kirchhoff–Neumann vertex condition at any  $v \in V^b \setminus \partial\Gamma^b$  and the Dirichlet boundary condition on  $\partial\Gamma^b$ , where  $\partial\Gamma^b$  be the boundary of  $\Gamma^b$ , namely,  $\partial\Gamma^b := \bigcup_{k \in \mathbb{Z}} (\overline{e_{0,1,k}} \cup \overline{e_{-1,3,k}} \cup \overline{e_{-1,4,k}} \cup \overline{e_{0,4,k}} \cup \overline{e_{0,5,k}} \cup \overline{e_{0,6,k}})$ . More precisely, the Kirchhoff–Neumann boundary conditions are

$$\begin{aligned} y_{n-1,2,k}(1) &= y_{n-1,3,k}(0) = y_{n,1,k}(0), \quad -y'_{n-1,2,k}(1) + y'_{n-1,3,k}(0) + y'_{n,1,k}(0) = 0 \text{ at } A_{n,k}, \\ y_{n,1,k}(1) &= y_{n,2,k}(0) = y_{n,6,k-1}(1), \quad -y'_{n,1,k}(1) + y'_{n,2,k}(0) - y'_{n,6,k-1}(1) = 0 \text{ at } B_{n,k}, \\ y_{n,5,k}(1) &= y_{n,6,k}(0) = y_{n+1,4,k}(0), \quad -y'_{n,5,k}(1) + y'_{n,6,k}(0) + y'_{n+1,4,k}(0) = 0 \text{ at } C_{n+1,k}, \\ y_{n,3,k}(1) &= y_{n,4,k}(1) = y_{n,5,k}(0), \quad -y'_{n,3,k}(1) - y'_{n,4,k}(1) + y'_{n,5,k}(0) = 0 \text{ at } D_{n,k} \end{aligned}$$

for  $(n,k) \in \mathbb{N} \times \mathbb{Z}$ . On the other hand, the Dirichlet boundary condition is expressed as  $y \equiv 0$  on  $\partial\Gamma^b$ . These boundary conditions make  $H^b$  self-adjoint.

Our operator  $H^b$  is not periodic in  $\mathbf{a}_1 := \overrightarrow{B_{0,1}B_{1,1}}$  but periodic in  $\mathbf{a}_2 := \overrightarrow{B_{0,1}B_{0,2}}$ . Thus, we give a direct integral decomposition to  $H^b$  in the direction  $\mathbf{a}_2$  [10]. For that purpose, we construct a fiber operator  $H^b(\mu)$  of  $H^b$ , where  $\mu \in S^1$  is a quasi-momentum. Put  $\mathcal{Z}_0 = \mathcal{Z}_{1,0} \cup \mathcal{Z}_{2,0} \cup \mathcal{Z}_{3,0}$ , where  $\mathcal{Z}_{1,0} = \mathbb{N} \times \mathcal{J}$ ,  $\mathcal{Z}_{2,0} = \{0\} \times \{0,2\}$ ,  $\mathcal{Z}_{3,0} = \{(0,1), (0,4), (0,5), (0,6), (-1,3), (-1,5)\}$ . Moreover, we define the funda-

mental domain  $\Gamma_0^\flat = (E_0^\flat, V_0^\flat)$  through

$$E_0^\flat = \{e_{n,j,0} \mid (n,j) \in \mathcal{Z}_0\}, \quad V_0^\flat = \left( \bigcup_{n \in \mathbb{N} \cup \{0\}} \{A_{n,0}, B_{n,0}, C_{n,0}, D_{n,0}\} \right) \cup \{D_{-1,0}\}.$$

Let  $\partial\Gamma_0^\flat = \bigcup_{(n,j) \in \mathcal{Z}_{3,0}} \overline{e_{n,j,0}}$ . Hereafter, we abbreviate  $e_{n,j,0}$  to  $e_{n,j}$  and apply the similar rule for  $y_{n,j,0}$  and  $A_{n,0}, B_{n,0}, C_{n,0}, D_{n,0}$ . We define the fiber operator  $H^b(\mu)$  in  $L^2(\Gamma_0)$  as

$$(H^b(\mu)y)_{n,j}(x) = -y''_{n,j}(x) + q(x)y_{n,j}(x), \quad x \in (0,1) \simeq e_{n,j}, \quad (n,j) \in \mathcal{Z}_0,$$

where  $y \in \text{dom}(H^b(\mu))$  is imposed the vertex conditions

$$y_{n-1,2}(1) = y_{n-1,3}(0) = y_{n,1}(0), \quad -y'_{n-1,2}(1) + y'_{n-1,3}(0) + y'_{n,1}(0) = 0 \text{ at } A_n, \quad (1.1)$$

$$y_{n,1}(1) = y_{n,2}(0) = e^{-i\mu}y_{n,6}(1), \quad -y'_{n,1}(1) + y'_{n,2}(0) - e^{-i\mu}y'_{n,6}(1) = 0 \text{ at } B_n, \quad (1.2)$$

$$y_{n,5}(1) = y_{n,6}(0) = y_{n+1,4}(0), \quad -y'_{n,5}(1) + y'_{n,6}(0) + y'_{n+1,4}(0) = 0 \text{ at } C_{n+1}, \quad (1.3)$$

$$y_{n,3}(1) = y_{n,4}(1) = y_{n,5}(0), \quad -y'_{n,3}(1) - y'_{n,4}(1) + y'_{n,5}(0) = 0 \text{ at } D_n \quad (1.4)$$

and the Dirichlet boundary condition  $y \equiv 0$  on  $\partial\Gamma_0^\flat$ . Put the direct integral decomposition  $\mathcal{H} := \int_{S^1}^\oplus L^2(\Gamma_0^\flat) \frac{d\mu}{2\pi}$  (see [6, 10] for the definition) and denote by  $L_{\text{comp}}^2(\Gamma^\flat)$  the set of all compactly supported function in  $L^2(\Gamma^\flat)$ . Then, the operator  $U : L_{\text{comp}}^2(\Gamma^\flat) \rightarrow \mathcal{H}$  acting as

$$(Uf)_\mu(x) = \sum_{m \in \mathbb{Z}} e^{-im\mu} f(x + m\mathbf{a}_2), \quad x \in \Gamma_0^\flat, \quad \mu \in S^1$$

is well-defined and is uniquely extended to the unitary operator  $U : L^2(\Gamma^\flat) \rightarrow \mathcal{H}$ . This operator yields the unitary equivalence

$$UH^bU^{-1} = \int_{S^1}^\oplus H^b(\mu) \frac{d\mu}{2\pi}$$

in a similar way to [6, 10]. Since  $\lambda \in \sigma(H^b)$  is characterize by  $\lambda \in \mathbb{R}$  satisfying  $m(\{\mu \in S^1 \mid \sigma(H^b(\mu)) \cap (\lambda - \varepsilon, \lambda + \varepsilon) \neq \emptyset\}) > 0$  for any  $\varepsilon > 0$  and the Lebesgue measure  $m$ , we hereafter study the spectrum of  $H^b(\mu)$ .

To state our main results, we need notations from the theory of the Hill operator  $L := -\frac{d^2}{dx^2} + q(x)$  in  $L^2(\mathbb{R})$  [2, 7, 10], where  $q$  is extended to be 1-periodic. For  $\lambda \in \mathbb{C}$ , let  $\theta(x, \lambda)$  and  $\varphi(x, \lambda)$  be the fundamental solutions to  $-y'' + qy = \lambda y$  on  $\mathbb{R}$  together with the initial conditions  $(\theta(0, \lambda), \theta'(0, \lambda)) = (1, 0)$  and  $(\varphi(0, \lambda), \varphi'(0, \lambda)) = (0, 1)$ , respectively. For our convenience, we use the abbreviations  $(\theta_1, \theta'_1, \varphi_1, \varphi'_1) = (\theta(1, \lambda), \theta'(1, \lambda), \varphi(1, \lambda), \varphi'(1, \lambda))$ . Then, the entire function  $\Delta(\lambda) = \frac{\theta_1 + \varphi'_1}{2}$  is known as the spectral discriminant of  $L$ . In [10], the result  $\sigma(L) = \sigma_{ac}(L) = \{\lambda \in \mathbb{R} \mid |\Delta(\lambda)| \leq 1\}$  is established by the theory of the direct integral decomposition of  $L$ . Furthermore, the function  $\Delta_-(\lambda) = \frac{\theta_1 - \varphi'_1}{2}$  determines if  $q$  is even in the sense of  $q(x) = q(1-x)$  on

$(0, 1)$ . The potential  $q$  is even if and only if  $\Delta_- \equiv 0$  (see [5, Lemma 3.1(iii)]). Moreover, we define  $\sigma_D$  as the set of all eigenvalues of the Dirichlet problem  $-y'' + qy = \lambda y$  on  $(0, 1)$  with the Dirichlet condition  $y(0) = y(1) = 0$ . This is characterized as  $\sigma_D = \{\lambda \in \mathbb{R} \mid \varphi(1, \lambda) = 0\}$ .

In this paper, we construct the spectral theory of  $H^b(\mu)$  from the point of view of the functions

$$D_s(\mu, \lambda) = d_s^2(\mu, \lambda) - 16 \sin^2 \frac{\mu}{4} \quad \text{and} \quad D_c(\mu, \lambda) = d_c^2(\mu, \lambda) - 16 \cos^2 \frac{\mu}{4}. \quad (1.5)$$

Here,  $d_s(\mu, \lambda)$  and  $d_c(\mu, \lambda)$  are defined as  $d_s(\mu, \lambda) = 9\Delta^2(\lambda) - \Delta_-^2(\lambda) - 1 - 4 \sin^2 \frac{\mu}{4}$  and  $d_c(\mu, \lambda) = 9\Delta^2(\lambda) - \Delta_-^2(\lambda) - 1 - 4 \cos^2 \frac{\mu}{4}$ . Moreover, we define

$$\begin{aligned} D_1 &:= \{\lambda \in \mathbb{R} \setminus \sigma_D \mid D_s(\mu, \lambda) < 0, \quad D_c(\mu, \lambda) < 0\}, \\ D_2 &:= \{\lambda \in \mathbb{R} \setminus \sigma_D \mid D_s(\mu, \lambda) < 0, \quad D_c(\mu, \lambda) > 0\}, \\ D_3 &:= \{\lambda \in \mathbb{R} \setminus \sigma_D \mid D_s(\mu, \lambda) > 0, \quad D_c(\mu, \lambda) < 0\}, \\ D_4 &:= \{\lambda \in \mathbb{R} \setminus \sigma_D \mid D_s(\mu, \lambda) > 0, \quad D_c(\mu, \lambda) > 0\} \end{aligned}$$

and give a decomposition  $D_4 = D_4^+ \cup D_4^-$ , where

$$\begin{aligned} D_4^+ &:= \left\{ \lambda \in \mathbb{R} \setminus \sigma_D \mid d_c(\mu, \lambda) > 4 \cos^2 \frac{\mu}{4}, \quad d_s(\mu, \lambda) > 4 \left| \sin \frac{\mu}{4} \right| \right\} \\ D_4^- &:= \left\{ \lambda \in \mathbb{R} \setminus \sigma_D \mid d_c(\mu, \lambda) < -4 \cos^2 \frac{\mu}{4}, \quad d_s(\mu, \lambda) < -4 \left| \sin \frac{\mu}{4} \right| \right\}. \end{aligned}$$

Our main results are stated as

**THEOREM 1.1.** *On the spectrum of the fiber operator  $H^b(\mu)$ , we have the followings:*

- (0) For any  $\mu \in S^1$ , we have  $\sigma_D \subset \sigma_p(H^b(\mu))$ .
- (1) If  $\mu \in S^1 \setminus \{0\}$ , then  $D_1 \subset \sigma(H^b(\mu))$ .
- (2) If  $\mu \in S^1 \setminus \{0\}$ , then  $D_2 \subset \sigma(H^b(\mu))$ .
- (3) If  $\mu \in S^1 \setminus \{0, \pm \frac{2}{3}\pi\}$ , then  $D_3 \subset \sigma(H^b(\mu))$ .
- (4) If  $\mu \in S^1 \setminus \{0, \pm \pi\}$ , then  $D_4^+ \subset \rho(H^b(\mu))$ .

To describe the statements on  $D_4^-$ , we put

$$m_{12}(\lambda) = \frac{\varphi_1(2\Delta + \varphi_1')}{1 - e^{-i\mu}}$$

for  $\mu \in S^1 \setminus \{0\}$ . If  $q$  is even, then we note that  $m_{12} = 0$  is equivalent to  $3\Delta + \Delta_- = 0$ .

**THEOREM 1.2.** *Assume that  $\mu \in S^1 \setminus \{0, \pm \frac{2}{3}\pi, \pm \pi\}$  and  $\lambda \in D_4^-$ .*

(A) *Assume that  $m_{12} \neq 0$  and  $3\Delta + \Delta_- = 0$ .*

- (1) *If  $\frac{2}{3}\pi < |\mu| < \pi$ , then  $\lambda \in \sigma_p(H^b(\mu))$ .*

(2) If  $0 < |\mu| < \frac{2}{3}\pi$ , then  $\lambda \in \rho(H^b(\mu))$ .

(B) Assume that  $m_{12} \neq 0$  and  $3\Delta + \Delta_- \neq 0$ .

(1) If  $d_s - \sqrt{D_s} + d_c - \sqrt{D_c} + 8 \neq 0$ , then  $\lambda \in \rho(H^b(\mu))$ .

(2) If  $d_s - \sqrt{D_s} + d_c - \sqrt{D_c} + 8 = 0$ , then  $\lambda \in \sigma_p(H^b(\mu))$ .

(C) Assume that  $m_{12} = 0$  and  $q$  is even. Then,  $3\Delta + \Delta_- = 0$  also holds true. If  $\frac{2}{3}\pi < |\mu| < \pi$ , then  $\lambda \in \sigma_p(H^b)$ . Otherwise,  $\lambda \in \rho(H^b(\mu))$ .

(D) If  $m_{12} = 0$  and  $q$  is not even, then  $\lambda \in \rho(H^b(\mu))$ .

Our main results relates the dispersion relation for almost every  $\mu \in S^1$  (except the case of  $D_s(\mu, \lambda) = 0$  and  $D_c(\mu, \lambda) = 0$ ). In order to draw the picture, we prepare the notations:

$$\ell_1(\mu) = \{\lambda \in D_4^- \mid d_s - \sqrt{D_s} + d_c - \sqrt{D_c} + 8 = 0\}.$$

$$\ell_2(\mu) = \{\lambda \in D_4^- \mid 3\Delta + \Delta_- = 0\}.$$

$$\mathcal{M}_1 = \left\{ (\lambda, \mu) \mid \lambda \in \ell_1(\mu), \quad \mu \in S^1 \setminus \left\{ 0, \pm \frac{2}{3}\pi, \pm\pi \right\} \right\}.$$

$$\mathcal{M}_2 = \left\{ (\lambda, \mu) \mid \lambda \in \ell_2(\mu), \quad \frac{2}{3}\pi < |\mu| < \pi \right\}.$$

Then, the picture of dispersion relation for  $q \equiv 0$  is seen in Fig. 3. The picture will help us to understand the statements of Theorem 1.1 and 1.2. If  $q$  is even,  $m_{12} = 0$  is equivalent to  $3\Delta + \Delta_- = 0$ . Thus, the eigenvalue curve  $3\Delta + \Delta_- = 0$  and  $m_{12} = 0$  in Fig. 3 overlaps each other in the case of  $q = 0$ .

Next, we would like to compare our results with [8]. In [8], spectral properties are studied for graphenes with standard zigzag boundaries. Let  $\Gamma^\sharp = (E^\sharp, V^\sharp)$  be the metric graph corresponding to the half space of the graphene seen in Fig. 4, where  $E^\sharp$  and  $V^\sharp$  are the set of edges and vertices respectively. Denote by  $H^\sharp$  the Schrödinger operator on  $\Gamma^\sharp$  with the Dirichlet boundary conditions on  $\partial\Gamma^\sharp$  and the Kirchhoff–Neumann vertex conditions at  $V^\sharp \setminus \partial\Gamma^\sharp$ . The operator  $H^\sharp$  acts as  $-\frac{d^2}{dx^2} + q$  on each  $(0, 1) \simeq e \in E^\sharp$ , where  $q$  is the same as the potential of  $H^b$ . Since there are no periodic bump on the boundaries, the fundamental domain of  $H^\sharp$  is half as large as the one of  $H^b$ . As a result, spectral discriminant  $D(\mu, \lambda)$  of the fiber operator  $H^\sharp(\mu)$  corresponding to  $H^\sharp$  can be simplified instead of (1.5) as

$$D(\mu, \lambda) = d^2(\mu, \lambda) - 16\cos^2 \frac{\mu}{2},$$

where  $d(\mu, \lambda) = 9\Delta^2(\lambda) - \Delta_-^2(\lambda) - 1 - 4\cos^2 \frac{\mu}{2}$  for  $\lambda \notin \sigma_D$  and  $\mu \in S^1 \setminus \{\pm\pi\}$ . This appears as in the explicit formulae of the eigenvalues

$$\rho_\pm = \frac{1}{2(1 + e^{-i\mu})} (d(\mu, \lambda) \pm \sqrt{D(\mu, \lambda)})$$

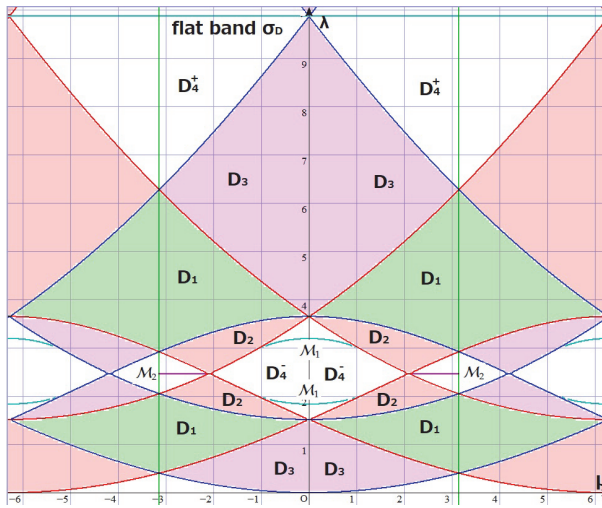


Fig. 3: The dispersion relation in the case of  $q \equiv 0$ .

of the transfer matrix  $M^\sharp(\lambda)$  defined as

$$\begin{pmatrix} y_{n+1,1,0}(0, \lambda) \\ y'_{n+1,1,0}(0, \lambda) \end{pmatrix} = M^\sharp(\lambda) \begin{pmatrix} y_{n,1,0}(0, \lambda) \\ y'_{n,1,0}(0, \lambda) \end{pmatrix}$$

for a solution  $y = (y_{n,j,k})$  on  $\Gamma^\sharp$  to  $H^\sharp(\mu)y = \lambda y$  and  $\lambda \in \mathbb{R} \setminus \sigma_D$ . Since  $M^\sharp(\lambda)$  is a  $2 \times 2$  matrix in contrast to the one for  $H^p$  (see (2.1) below), it is relatively easier to find the eigenspace of  $V(\rho_\pm)$ . Prepare the key vector  $\mathbf{e} = \begin{pmatrix} 0 & 1 \end{pmatrix}^\top$ . Then, the function  $D(\mu, \lambda)$  plays the role of a spectral discriminant:

**THEOREM 1.3.** (Theorem 2.3 in [8]) Assume that  $\lambda \in \mathbb{R} \setminus \sigma_D$  and  $\mu \in S^1 \setminus \{\pm\pi\}$ .

- (I) If  $D(\mu, \lambda) < 0$ , then we have  $|\rho_\pm| = 1$ ,  $\lambda \in \sigma(H^\sharp(\mu))$  and  $\lambda \notin \sigma_p(H^\sharp(\mu))$ .
- (II) If  $D(\mu, \lambda) > 0$ , then we have  $\rho_+ \overline{\rho_-} = 1$ ,  $|\rho_\pm| \neq 1$  and the followings:
  - (i) If  $\mathbf{e} \notin V(\rho_+)$  and  $\mathbf{e} \notin V(\rho_-)$ , then we have  $\lambda \in \rho(H^\sharp(\mu))$ .
  - (ii) Assume that  $\mathbf{e} \in V(\rho_+)$ . If  $|\rho_+| < 1$ , then we have  $\lambda \in \sigma_p(H^\sharp(\mu))$ . Otherwise, namely, if  $|\rho_+| > 1$ , then we have  $\lambda \in \rho(H^\sharp(\mu))$ .
  - (iii) Assume that  $\mathbf{e} \in V(\rho_-)$ . If  $|\rho_+| > 1$ , then we have  $\lambda \in \sigma_p(H^\sharp(\mu))$ . Otherwise, namely, if  $|\rho_+| < 1$ , then we have  $\lambda \in \rho(H^\sharp(\mu))$ .

The signature of the discriminant  $D(\mu, \lambda)$  is related in determining whether or not  $\lambda \notin \sigma_D$  belongs to the spectrum of the fiber operator  $H^\sharp(\mu)$ . In this sense, our results

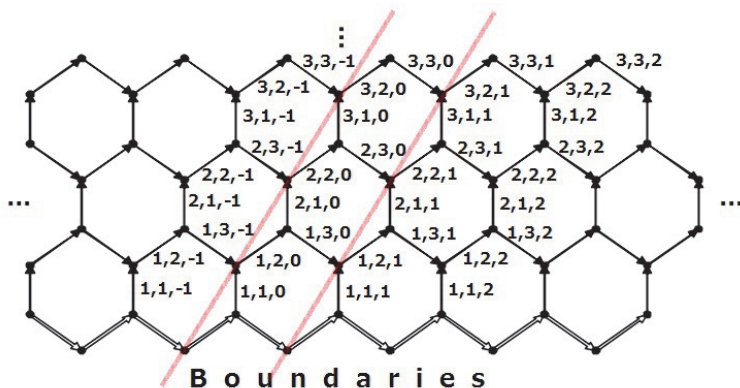


Fig. 4: Graphene with standard zigzag boundaries

in this paper (Theorems 1.1 and 1.2) are analogues of Theorem 1.3. In the case without bumpy boundaries,  $D(\mu, \lambda) < 0$  is equivalent to  $|F(\mu, \lambda)| < 1$ , where

$$F(\mu, \lambda) = \frac{1}{4 \cos \frac{\mu}{2}} \left( 9\Delta^2(\lambda) - \Delta_-^2(\lambda) - 1 - 4 \cos^2 \frac{\mu}{2} \right).$$

Since the asymptotics of  $\theta_1$  and  $\varphi'_1$  are well-known in [9], the behavior of the function  $F(\mu, \lambda)$  can be stated in §3 in [8]. As a result, we constructed the spectral band-gap structure of  $H^\sharp(\mu)$  and  $H^\sharp$ . In the case of  $D(\mu, \lambda) > 0$ ,  $\lambda \in \mathbb{R} \setminus \sigma_D$  and  $\mu \in S^1 \setminus \{\pm\pi\}$ , the conditions  $\mathbf{e} \in V(\rho_+)$  and  $|\rho_+| > 1$  hold true in the case of  $\mu \in (-\pi, -\frac{2}{3}\pi) \cup (\frac{2}{3}\pi, \pi)$  and  $m_{12}^\sharp(\lambda) = 0$ , where  $M^\sharp(\lambda) = (m_{ij}^\sharp(\lambda))_{i,j=1,2}$  (see [8, Theorem 2.7]). The variety defined by  $m_{12}^\sharp(\lambda) = 0$  and  $\mu \in (-\pi, -\frac{2}{3}\pi) \cup (\frac{2}{3}\pi, \pi)$  appears as eigenvalue curves in spectral gaps of  $H^\sharp(\mu)$  (see Fig. 5). For  $\lambda \notin \sigma_D$ , the three conditions  $m_{12}^\sharp(\lambda) = 0$ ,  $m_{12}(\lambda) = 0$  and  $\theta_1 + 2\varphi'_1 = 0$  are equivalent. Compared with Fig. 3, it looks like there are no difference for eigenvalue curves  $\theta_1 + 2\varphi'_1 = 0$  ( $\mu \in (-\pi, -\frac{2}{3}\pi) \cup (\frac{2}{3}\pi, \pi)$ ). The difference between the eigenvalue curves of  $H^\sharp(\mu)$  and  $H^b(\mu)$  appears as the varieties  $\mathcal{M}_1$ . In the case of  $H^b(\mu)$ , the eigenvalue curve is defined as  $3\Delta + \Delta_- = 0$  and  $\mu \in (-\pi, -\frac{2}{3}\pi) \cup (\frac{2}{3}\pi, \pi)$ . Note that the condition  $3\Delta + \Delta_- = 0$  is equivalent to  $2\theta_1 + \varphi'_1 = 0$ .

Let us introduce the content of this paper and explain how new our approach in this study is. In this paper, we deeply rely on the Cramer's rule for our spectral analysis of the fiber operator  $H^b(\mu)$ . In Section 2, we study the spectral properties of a transfer matrix  $M(\lambda)$  for  $H^b(\mu)$  defined in (2.1). In principle, a non-trivial solution  $y$  to  $H^b y = \lambda y$  for  $\lambda \in \mathbb{R} \setminus \sigma_D$  can be written explicitly. However, it is more complicated to find the components of the  $4 \times 4$  matrix because the size of the fundamental domain of  $\Gamma^b$



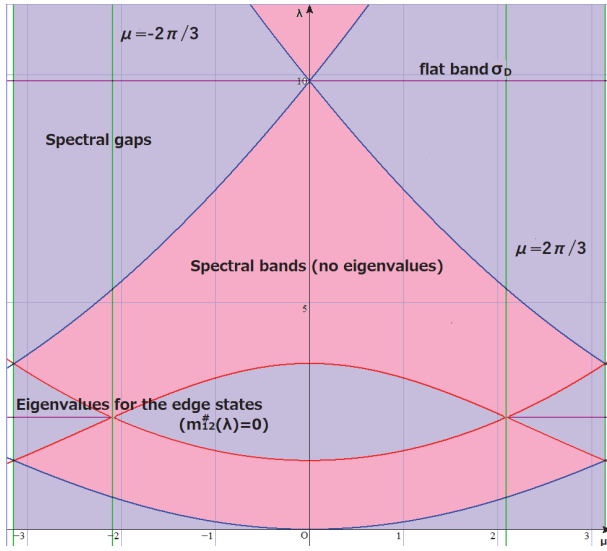


Fig. 5: The dispersion relation to  $H^\sharp$  in the unperturbed case  $q \equiv 0$

is twice as big as the one of  $\Gamma^\sharp$ . The first highlight is the block matrix form

$$M(\lambda) = \begin{pmatrix} A & e^{-i\mu}B \\ B & A \end{pmatrix} \quad (1.6)$$

(see Lemma 2.1). This helps us to calculate the eigenvalues  $\rho_s^\pm, \rho_c^\pm$  of the transfer matrix  $M(\lambda)$  and the corresponding eigenspaces  $V(\rho_s^\pm)$  and  $V(\rho_c^\pm)$ . In Lemma 2.4, the eigenvectors in  $V(\rho_\bullet^\pm)$  are explicitly written for each  $\bullet = s, c$ . In the subsection 3.1, we find fundamental solutions to  $H^b(\mu)y = \lambda y$ . In the case of  $\lambda \in \mathbb{R} \setminus \sigma_D$ , the fundamental solutions  $p$  and  $q$  to  $H^b(\mu)y = \lambda y$  as well as initial conditions  $p_{0,2}(0, \lambda) = 0$ ,  $p'_{0,2}(0, \lambda) = 1$ ,  $q_{1,4}(0, \lambda) = 0$ ,  $q'_{1,4}(0, \lambda) = 1$  are explicitly written as in Lemma 3.4 (2). As a result, we derive an explicit expression of a non-trivial solution  $y = (y_{n,j})_{(n,j) \in \mathcal{Z}_0}$  to  $H^b(\mu)y = \lambda y$  as well as the initial condition

$$\begin{pmatrix} y_{1,1}(0, \lambda) \\ y'_{1,1}(0, \lambda) \\ y_{1,4}(0, \lambda) \\ y'_{1,4}(0, \lambda) \end{pmatrix} = c_1 \begin{pmatrix} \varphi_1 \\ 2\Delta \\ 0 \\ 0 \end{pmatrix} + c_2 \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \quad (1.7)$$

with constants  $(c_1, c_2) \in \mathbb{C}^2 \setminus \{(0, 0)\}$ . As in Lemma 3.4 (1), the expression includes the eigenvalues  $\rho_c^\pm$  and  $\rho_s^\pm$  such as

$$\begin{aligned} y_{n,j}(x, \lambda) = & (\rho_c^+)^{n-1} (c_1 \eta_{j,1,c}^+ + c_2 \eta_{j,2,c}^+) + (\rho_c^-)^{n-1} (c_1 \eta_{j,1,c}^- + c_2 \eta_{j,2,c}^-) \\ & + (\rho_s^+)^{n-1} (c_1 \eta_{j,1,s}^+ + c_2 \eta_{j,2,s}^+) + (\rho_s^-)^{n-1} (c_1 \eta_{j,1,s}^- + c_2 \eta_{j,2,s}^-). \end{aligned}$$

Here,  $\eta_{j,\ell,\bullet}^{\pm} = \eta_{j,\ell,\bullet}^{\pm}(x, \lambda)$  is explicitly written as a linear combination of  $\theta(x, \lambda)$  and  $\varphi(x, \lambda)$  for  $j = 1, 2, 3, 4, 5, 6$ ,  $\ell = 1, 2$  and  $\bullet = s, c$ . Its coefficients  $\alpha_{j,\ell,\bullet}^{\pm}$  and  $\beta_{j,\ell,\bullet}^{\pm}$  is given in (3.7)–(3.9) by considering the eigenvector expansion (3.6) of the vectors  $\mathbf{e}_1$  and  $\mathbf{e}_2$  appering the initial condition (see (3.1)). In the subsection 3.2, we construct infinitely many linearly independent eigenfunctions to the eigenvalue  $\lambda \in \sigma_D$  with the help of the idea in [5]. Recall that  $\lambda \in \sigma_D$  is called a flat band. In section 4, we give the proof of Theorems 1.1 and 1.2. Assume that  $\lambda \in \mathbb{R} \setminus \sigma_D$ . In accordance with the signature of  $D_s(\mu, \lambda)$  and  $D_c(\mu, \lambda)$ , we have three classes  $|\rho_{\bullet}^{\pm}| = 1$ ,  $|\rho_{\bullet}^{\pm}| > 1$  and  $|\rho_{\bullet}^{\pm}| < 1$  for each symbol  $\bullet = s, c$ . In the case of  $D_s(\mu, \lambda) < 0$  and  $D_c(\mu, \lambda) < 0$ , the absolute value of all eigenvalues are 1:  $|\rho_s^{\pm}| = |\rho_c^{\pm}| = 1$ . So, we see that  $\|y_{n,j}\|_{L^2(0,1)}^2$  is uniformly bounded with respect to  $n \in \mathbb{N}$  and any  $j$ . Then, we see that all non-trivial solution  $y$  is a generalized eigenfunction for  $\lambda \in D_1$ . This is the simplest case in the classifications  $\{D_j\}_{j=1,2,3,4}$ . For example, the case of  $\lambda \in D_2$  is more complicated because  $\|y_{n,j}\|_{L^2(0,1)}$  might grow exponentially as  $n \rightarrow \infty$  due to  $|\rho_s^{\pm}| = 1$ ,  $|\rho_c^{-}| > 1$  and  $|\rho_c^{+}| < 1$  (see Lemma 4.1). If there exists some pair  $(c_1, c_2) \in \mathbb{C}^2 \setminus \{(0, 0)\}$  satisfying  $c_1 \eta_{j,1,c}^{-}(x, \lambda) + c_2 \eta_{j,2,c}^{-}(x, \lambda) \equiv 0$ , namely,  $(c_1 \alpha_{j,1,c}^{-} + c_1 \alpha_{j,2,c}^{-}, c_1 \beta_{j,1,c}^{-} + c_2 \beta_{j,2,c}^{-}) = (0, 0)$  for all  $j = 1, 2, 3, 4, 5, 6$ , then  $\|y_{n,j}\|_{L^2(0,1)}$  is uniformly bounded with respect to  $n \in \mathbb{N}$  and  $j$ . The coefficients  $\alpha_{j,1,c}^{-}, \alpha_{j,2,c}^{-}, \beta_{j,1,c}^{-}, \beta_{j,2,c}^{-}$  are appearing in the vectors  $\mathbf{e}_{1,s}^{-}$  and  $\mathbf{e}_{2,s}^{-}$  (see (3.7)–(3.9)). There exist unique constants  $\gamma_s^{-}, \delta_s^{-} \in \mathbb{C}$  such that  $\mathbf{e}_{1,s}^{-} = \gamma_s^{-} \mathbf{w}_s^{-}$  and  $\mathbf{e}_{2,s}^{-} = \delta_s^{-} \mathbf{w}_s^{-}$  because  $V(\rho_s^{\pm}) = \langle \mathbf{w}_s^{\pm} \rangle$ . As a result, we have  $\delta_c^{-} \alpha_{j,1,c}^{-} + (-\gamma_c^{-}) \alpha_{j,2,c}^{-} = 0$  and  $\delta_c^{-} \beta_{j,1,c}^{-} + (-\gamma_c^{-}) \beta_{j,2,c}^{-} = 0$ . To find  $(\delta_c^{-}, \gamma_c^{-}) \neq (0, 0)$ , we wonder to find the coefficients in the eigenvector expansion (4.2) and (4.3). However, this is very heavy task. Thus, we utilize the Cramer's rule. As a result, we derive a generalized eigenfunction for  $\lambda \in D_2$ .

## 2. Transfer matrix for the fiber operator $H^b(\mu)$

We pick  $y = (y_{n,j})_{(n,j) \in \mathcal{Z}_0} \in \text{dom}(H^b(\mu))$ , arbitrarily. Let us study the  $4 \times 4$  transfer matrix  $M(\lambda) = (m_{ij}(\lambda))$  defined as

$$\begin{pmatrix} y_{n+1,1}(0, \lambda) \\ y'_{n+1,1}(0, \lambda) \\ y_{n+1,4}(0, \lambda) \\ y'_{n+1,4}(0, \lambda) \end{pmatrix} = M(\lambda) \begin{pmatrix} y_{n,1}(0, \lambda) \\ y'_{n,1}(0, \lambda) \\ y_{n,4}(0, \lambda) \\ y'_{n,4}(0, \lambda) \end{pmatrix} \quad (n \in \mathbb{N}) \quad (2.1)$$

and find its eigenvalues  $\rho_s^{\pm}$  and  $\rho_c^{\pm}$  by making use of the block matrix.

LEMMA 2.1. *Let  $\mu \in S^1 \setminus \{0\} = [-\pi, 0) \cup (0, \pi)$  and  $\lambda \in \mathbb{R} \setminus \sigma_D$ . Then, we have*

$$m_{11} = \frac{\theta'_1 \varphi_1 + 2\Delta \theta_1}{1 - e^{-i\mu}} \quad \text{and} \quad m_{12} = \frac{\varphi_1 \varphi'_1 + 2\Delta \varphi_1}{1 - e^{-i\mu}}.$$

Furthermore,  $M(\lambda)$  has the block matrix form (1.6), where

$$A = \begin{pmatrix} m_{11} & m_{12} \\ \frac{2\Delta m_{11} - \theta_1}{\varphi_1} & -1 + \frac{2\Delta m_{12}}{\varphi_1} \end{pmatrix}$$

and

$$B = \begin{pmatrix} -m_{11} & -m_{12} \\ \frac{-2\Delta m_{11} - \theta_1 e^{i\mu}}{\varphi_1} & -e^{i\mu} - \frac{2\Delta m_{12}}{\varphi_1} \end{pmatrix}.$$

*Proof.* Putting  $\alpha_n = y_{n,1}(0, \lambda)$ ,  $\alpha'_n = y'_{n,1}(0, \lambda)$ ,  $\beta_n = y_{n,2}(0, \lambda)$ ,  $\gamma_n = y_{n,4}(0, \lambda)$ ,  $\gamma'_n = y'_{n,4}(0, \lambda)$ ,  $\delta_n = y_{n,5}(0, \lambda)$ , we have

$$\begin{cases} y_{n,1}(x, \lambda) = \alpha_n \theta(x, \lambda) + \alpha'_n \varphi(x, \lambda), \\ y_{n,2}(x, \lambda) = \beta_n \theta(x, \lambda) + y'_{n,2}(0, \lambda) \varphi(x, \lambda), \\ y_{n,3}(x, \lambda) = \alpha_{n+1} \theta(x, \lambda) + y'_{n,3}(0, \lambda) \varphi(x, \lambda), \\ y_{n,4}(x, \lambda) = \gamma_n \theta(x, \lambda) + \gamma'_n \varphi(x, \lambda), \\ y_{n,5}(x, \lambda) = \delta_n \theta(x, \lambda) + y'_{n,5}(0, \lambda) \varphi(x, \lambda), \\ y_{n,6}(x, \lambda) = \gamma_{n+1} \theta(x, \lambda) + y'_{n,6}(0, \lambda) \varphi(x, \lambda) \end{cases} \quad (2.2)$$

due to  $y_{n,j}(x, \lambda) = y_{n,j}(0, \lambda) \theta(x, \lambda) + y'_{n,j}(0, \lambda) \varphi(x, \lambda)$  on  $e_{n,j}$  for  $(n, j) \in \mathcal{Z}_0$ . Substituting these (1.2) and (1.4), we have

$$-(\alpha_n \theta'_1 + \alpha'_n \varphi'_1) + y'_{n,2}(0, \lambda) - e^{-i\mu} (\gamma_{n+1} \theta'_1 + y'_{n,6}(0, \lambda) \varphi'_1) = 0, \quad (2.3)$$

$$-(\alpha_{n+1} \theta'_1 + y'_{n,3}(0, \lambda) \varphi'_1) - (\gamma_n \theta'_1 + \gamma'_n \varphi'_1) + y'_{n,5}(0, \lambda) = 0. \quad (2.4)$$

Note that  $y'_{n,j}(0, \lambda) = (y_{n,j}(1, \lambda) - \theta_1 y_{n,j}(0, \lambda)) / \varphi_1$  yields

$$y'_{n,2}(0, \lambda) = \frac{\alpha_{n+1} - \theta_1 \beta_n}{\varphi_1}, \quad y'_{n,6}(0, \lambda) = \frac{e^{i\mu} \beta_n - \theta_1 \gamma_{n+1}}{\varphi_1}, \quad (2.5)$$

$$y'_{n,3}(0, \lambda) = \frac{\delta_n - \theta_1 \alpha_{n+1}}{\varphi_1}, \quad y'_{n,5}(0, \lambda) = \frac{\gamma_{n+1} - \theta_1 \delta_n}{\varphi_1}. \quad (2.6)$$

Substituting these into (2.3) and (2.4), we have

$$\begin{aligned} \alpha_{n+1} + e^{-i\mu} \gamma_{n+1} &= \alpha_n \theta'_1 \varphi_1 + \alpha'_n \varphi_1 \varphi'_1 + 2\Delta \beta_n, \\ \alpha_{n+1} + \gamma_{n+1} &= \gamma_n \theta'_1 \varphi_1 + \gamma'_n \varphi_1 \varphi'_1 + 2\Delta \delta_n \end{aligned}$$

using  $\theta_1 \varphi'_1 - \theta'_1 \varphi_1 = 1$  and  $\theta_1 + \varphi'_1 = 2\Delta$ . Substituting  $\beta_n = y_{n,1}(1, \lambda) = \alpha_n \theta_1 + \alpha'_n \varphi_1$  and  $\delta_n = y_{n,4}(1, \lambda) = \gamma_n \theta_1 + \gamma'_n \varphi_1$  into these, we derive

$$\begin{aligned} \alpha_{n+1} + e^{-i\mu} \gamma_{n+1} &= \alpha_n (\theta'_1 \varphi_1 + 2\Delta \theta_1) + \alpha'_n (\varphi_1 \varphi'_1 + 2\Delta \varphi_1), \\ \alpha_{n+1} + \gamma_{n+1} &= \gamma_n (\theta'_1 \varphi_1 + 2\Delta \theta_1) + \gamma'_n (\varphi_1 \varphi'_1 + 2\Delta \varphi_1). \end{aligned}$$

These yields

$$\begin{aligned} &(1 - e^{-i\mu}) \alpha_{n+1} \\ &= \alpha_n (\theta'_1 \varphi_1 + 2\Delta \theta_1) + \alpha'_n (\varphi_1 \varphi'_1 + 2\Delta \varphi_1) - e^{-i\mu} \{ \gamma_n (\theta'_1 \varphi_1 + 2\Delta \theta_1) + \gamma'_n (\varphi_1 \varphi'_1 + 2\Delta \varphi_1) \}, \\ &(1 - e^{-i\mu}) \gamma_{n+1} \\ &= -\alpha_n (\theta'_1 \varphi_1 + 2\Delta \theta_1) - \alpha'_n (\varphi_1 \varphi'_1 + 2\Delta \varphi_1) + \gamma_n (\theta'_1 \varphi_1 + 2\Delta \theta_1) + \gamma'_n (\varphi_1 \varphi'_1 + 2\Delta \varphi_1). \end{aligned}$$

Hence, we have

$$m_{11} = m_{33} = \frac{\theta'_1 \varphi_1 + 2\Delta\theta_1}{1 - e^{-i\mu}}, \quad m_{12} = m_{34} = \frac{\varphi_1 \varphi'_1 + 2\Delta\varphi_1}{1 - e^{-i\mu}},$$

$m_{13} = -e^{-i\mu}m_{11}$ ,  $m_{14} = -e^{-i\mu}m_{12}$ ,  $m_{31} = -m_{11}$ ,  $m_{32} = -m_{12}$ . Thus, it turns out that the components of the 1st and 3rd rows of  $M(\lambda)$  are written as in the desired statement.

Next, we find the components of the 2nd and 4th rows of  $M(\lambda)$ . Substituting (2.2) into (1.1) and (1.3), we have

$$\begin{aligned} \alpha'_{n+1} &= y'_{n,2}(1, \lambda) - y'_{n,3}(0, \lambda) = (\beta_n \theta'_1 + y'_{n,2}(0, \lambda) \varphi'_1) - y'_{n,3}(0, \lambda), \\ \gamma'_{n+1} &= y'_{n+1,4}(0, \lambda) = y'_{n,5}(1, \lambda) - y'_{n,6}(0, \lambda) = (\delta_n \theta'_1 + y'_{n,5}(0, \lambda) \varphi'_1) - y'_{n,6}(0, \lambda). \end{aligned}$$

Inserting (2.5) and (2.6) into these, we obtain

$$\begin{aligned} \alpha'_{n+1} &= \frac{2\Delta m_{11} - \theta_1}{\varphi_1} \alpha_n + \left(-1 + \frac{2\Delta m_{12}}{\varphi_1}\right) \alpha'_n + \frac{2\Delta m_{13} - \theta_1}{\varphi_1} \gamma_n + \left(-1 + \frac{2\Delta m_{14}}{\varphi_1}\right) \gamma'_n, \\ \gamma'_{n+1} &= \frac{2\Delta m_{31} - \theta_1 e^{i\mu}}{\varphi_1} \alpha_n + \left(-e^{i\mu} + \frac{2\Delta m_{32}}{\varphi_1}\right) \alpha'_n + \frac{2\Delta m_{33} - \theta_1}{\varphi_1} \gamma_n + \left(-1 + \frac{2\Delta m_{34}}{\varphi_1}\right) \gamma'_n. \end{aligned}$$

These combined with  $m_{33} = m_{11}$ ,  $m_{34} = m_{12}$ ,  $m_{13} = -e^{-i\mu}m_{11}$ ,  $m_{14} = -e^{-i\mu}m_{12}$ ,  $m_{31} = -m_{11}$ ,  $m_{32} = -m_{12}$  give us the components of the 2nd and 4th rows of  $M(\lambda)$  in the desired form.  $\square$

Next, we calculate the eigenvalues of  $M(\lambda)$ . Since  $M(\lambda)$  is the  $4 \times 4$  matrix, it looks like difficult to achieve the calculation. However, the block form of  $M(\lambda)$  in Lemma 2.1 helps us to carry out the calculation:

LEMMA 2.2. Assume that  $\mu \in S^1 \setminus \{0\}$  and  $\lambda \in \mathbb{R} \setminus \sigma_D$ . Then, the eigenvalues of  $M(\lambda)$  are given by

$$\rho_s^\pm = \frac{d_s(\mu, \lambda) \pm \sqrt{D_s(\mu, \lambda)}}{4ie^{-\frac{i\mu}{4}} \sin \frac{\mu}{4}} \quad \text{and} \quad \rho_c^\pm = \frac{d_c(\mu, \lambda) \pm \sqrt{D_c(\mu, \lambda)}}{4e^{-\frac{i\mu}{4}} \cos \frac{\mu}{4}}.$$

*Proof.* Let  $E_n$  be the unit matrix of size  $n$  and consider the characteristic equation  $\det(\rho E_4 - M(\lambda)) = 0$ . Our first calculation is

$$\begin{aligned} \det(\rho E_4 - M(\lambda)) &= \begin{vmatrix} \rho E_2 - A & -e^{-i\mu} B \\ -B & \rho E_2 - A \end{vmatrix} \\ &= \begin{vmatrix} \rho E_2 - A - e^{-\frac{i\mu}{2}} B & -e^{-i\mu} B + e^{-\frac{i\mu}{2}} (\rho E_2 - A) \\ -B & \rho E_2 - A \end{vmatrix} \\ &= \begin{vmatrix} \rho E_2 - A - e^{-\frac{i\mu}{2}} B & O \\ -B & \rho E_2 - A + e^{-\frac{i\mu}{2}} B \end{vmatrix} \\ &= \det(\rho E_2 - A - e^{-\frac{i\mu}{2}} B) \det(\rho E_2 - A + e^{-\frac{i\mu}{2}} B). \end{aligned}$$

Since the components of  $A$  and  $B$  are found in Lemma 2.1, we have

$$\det(\rho E_2 - A - e^{-\frac{i\mu}{2}} B) = \rho^2 + \frac{(1 + e^{\frac{i\mu}{2}})(1 + e^{-\frac{i\mu}{2}}) - (8\Delta^2 + \theta'_1 \varphi_1)}{1 + e^{-\frac{i\mu}{2}}} \rho + \frac{1 + e^{\frac{i\mu}{2}}}{1 + e^{-\frac{i\mu}{2}}},$$

$$\det(\rho E_2 - A + e^{-\frac{i\mu}{2}} B) = \rho^2 + \frac{(1 - e^{\frac{i\mu}{2}})(1 - e^{-\frac{i\mu}{2}}) - (8\Delta^2 + \theta'_1 \varphi_1)}{1 - e^{-\frac{i\mu}{2}}} \rho + \frac{1 - e^{\frac{i\mu}{2}}}{1 - e^{-\frac{i\mu}{2}}}.$$

Now, we have the following elemental results:

$$1 + e^{-\frac{i\mu}{2}} = 1 + \cos \frac{\mu}{2} - i \sin \frac{\mu}{2} = 2 \cos^2 \frac{\mu}{4} - 2i \sin \frac{\mu}{4} \cos \frac{\mu}{4} = 2e^{-\frac{i\mu}{4}} \cos \frac{\mu}{4} (\neq 0),$$

$$1 - e^{-\frac{i\mu}{2}} = 1 - \cos \frac{\mu}{2} + i \sin \frac{\mu}{2} = 2 \sin^2 \frac{\mu}{4} + 2i \sin \frac{\mu}{4} \cos \frac{\mu}{4} = 2ie^{-\frac{i\mu}{4}} \sin \frac{\mu}{4} (\neq 0).$$

Using these 4 results, we obtain

$$\det(\rho E_2 - A - e^{-\frac{i\mu}{2}} B) = \rho^2 + \frac{4 \cos^2 \frac{\mu}{4} - 8\Delta^2 - \theta'_1 \varphi_1}{2e^{-\frac{i\mu}{4}} \cos \frac{\mu}{4}} \rho + e^{\frac{i\mu}{2}},$$

$$\det(\rho E_2 - A + e^{-\frac{i\mu}{2}} B) = \rho^2 + \frac{4 \sin^2 \frac{\mu}{4} - 8\Delta^2 - \theta'_1 \varphi_1}{2ie^{-\frac{i\mu}{4}} \sin \frac{\mu}{4}} \rho - e^{\frac{i\mu}{2}}.$$

The quadratic formula yields the eigenvalues  $\rho = \rho_s^\pm, \rho_c^\pm$  of  $M(\lambda)$ .  $\square$

Put  $S = \{\rho_s^+, \rho_s^-\} \cap \{\rho_c^+, \rho_c^-\}$ . In the next lemma, we examine if the eigenvalues of  $M(\lambda)$  are simple or not. For the most part, they are simple:

LEMMA 2.3. *For almost every  $\mu \in S^1$  and  $\lambda \in \mathbb{R}$ , we have  $S = \emptyset$ :*

- (1) *For any  $\mu \in S^1 \setminus \{0\}$ , we have  $S = \emptyset$  for almost every  $\lambda \in D_1$ .*
- (2) *For any  $\mu \in S^1 \setminus \{0\}$ , we have  $S = \emptyset$  for every  $\lambda \in D_2$ .*
- (3) *For any  $\mu \in S^1 \setminus \{0, \pm \frac{2}{3}\pi\}$ , we have  $S = \emptyset$  for every  $\lambda \in D_3$ .*
- (4) *For any  $\mu \in S^1 \setminus \{0\}$ , we have  $S = \emptyset$  for every  $\lambda \in D_4$ .*

*Proof.* (1) Assume that  $\rho_s^+ = \rho_c^\pm$ . Hence, we derive

$$\frac{d_s(\mu, \lambda)}{\sin \frac{\mu}{4}} = \mp \frac{\sqrt{-D_c(\mu, \lambda)}}{\cos \frac{\mu}{4}}, \quad -\frac{\sqrt{-D_s(\mu, \lambda)}}{\sin \frac{\mu}{4}} = \frac{d_c(\mu, \lambda)}{\cos \frac{\mu}{4}}.$$

This yields  $D_s(\mu, \lambda)D_c(\mu, \lambda) = d_s^2(\mu, \lambda)d_c^2(\mu, \lambda)$ . Put  $d = d(\lambda) = 9\Delta^2 - \Delta^2 - 1$ . Substituting  $D_s(\mu, \lambda) = d_s^2(\mu, \lambda) - 16\sin^2 \frac{\mu}{4}$  and  $D_c(\mu, \lambda) = d_c^2(\mu, \lambda) - 16\cos^2 \frac{\mu}{4}$ , we have  $d(d - 16\sin^2 \frac{\mu}{4} \cos^2 \frac{\mu}{4}) = 0$ . The asymptotic  $d(\lambda) \sim 9\cos^2 \sqrt{\lambda} - 1$  as  $|\lambda| \rightarrow \infty$  implies that the set  $L_1 := \{\lambda \in D_1 \mid d(d - 16\sin^2 \frac{\mu}{4} \cos^2 \frac{\mu}{4}) = 0\}$  has the Lebesgue measure 0 for each  $\mu \in S^1 \setminus \{0\}$ . So, we have  $\{\rho_s^+\} \cap \{\rho_c^+, \rho_c^-\} = \emptyset$  for almost every  $\lambda \in D_1$ . Similarly, we obtain  $\{\rho_s^-\} \cap \{\rho_c^+, \rho_c^-\} = \emptyset$  for almost every  $\lambda \in D_1$ .

(2) We shall show  $\rho_s^+ \neq \rho_c^+$ ,  $\rho_c^-$  by contradiction. Seeking a contradiction, we assume  $\rho_s^+ = \rho_c^\pm$ . Then, we have  $d_s = 0$  and

$$\frac{\sqrt{-D_s}}{\sin \frac{\mu}{4}} = \frac{d_c \pm \sqrt{D_c}}{\cos \frac{\mu}{4}}. \quad (2.7)$$

First, we consider the case of  $\mu \in (0, \pi)$ . Then,  $d_s = 0$  implies that  $\sqrt{-D_s} = 4 \sin \frac{\mu}{4}$ . Substituting this into (2.7), we have  $4 \cos \frac{\mu}{4} - d_c = \pm \sqrt{D_c}$ . This squared yields  $d_c = 4 \cos \frac{\mu}{4}$ . On the other hand, we have  $d_c = d_c - d_s = 4 \sin^2 \frac{\mu}{4} - 4 \cos^2 \frac{\mu}{4}$  because of  $d_s = 0$ . These results yield  $2 \cos^2 \frac{\mu}{4} + \cos \frac{\mu}{4} - 1 = 0$ . However, this does not have any root in  $(0, \pi)$ . Next, we consider the case of  $\mu \in [-\pi, 0)$ . By similar procedure, we arrive at  $2 \cos^2 \frac{\mu}{4} - \cos \frac{\mu}{4} - 1 = 0$ . This does not have any root in  $[-\pi, 0)$ . Thus, we have  $\rho_s^+ \neq \rho_c^+$ ,  $\rho_c^-$ . Since we also have  $\rho_s^- \neq \rho_c^\pm$  in a similar way, we derive  $S = \emptyset$ . The proof of (3) is similar to the one of (2).

(4) We shall show  $\rho_s^+ \neq \rho_c^+$ ,  $\rho_c^-$  by contradiction. Seeking a contradiction, we assume  $\rho_s^+ = \rho_c^\pm$ . Taking part of the real part and imaginary part of the equality, we have  $d_s(\mu, \lambda) + \sqrt{D_s(\mu, \lambda)} = 0$  and  $d_c(\mu, \lambda) \pm \sqrt{D_c(\mu, \lambda)} = 0$ . These mean that  $d_s^2 = d_s^2 - 16 \sin^2 \frac{\mu}{4}$  and  $d_c^2 = d_c^2 - 16 \cos^2 \frac{\mu}{4}$ , which yield a contradiction  $\sin \frac{\mu}{4} = \cos \frac{\mu}{4} = 0$ . Similarly, we have  $\rho_s^- \neq \rho_c^\pm$ . So,  $S = \emptyset$ .  $\square$

LEMMA 2.4. Assume that  $\mu \in S^1 \setminus \{0\}$ ,  $\lambda \in \mathbb{R} \setminus \sigma_D$  and  $S = \emptyset$ . Then, there exists some  $\mathbf{x}_c^\pm$  and  $\mathbf{x}_s^\pm \in \mathbb{C}^2$  such that  $V(\rho_c^\pm) = \langle \mathbf{w}_c^\pm \rangle$  and  $V(\rho_s^\pm) = \langle \mathbf{w}_s^\pm \rangle$ , where

$$\mathbf{w}_c^\pm = \begin{pmatrix} \mathbf{x}_c^\pm \\ e^{\frac{i\mu}{2}} \mathbf{x}_c^\pm \end{pmatrix}, \quad \mathbf{w}_s^\pm = \begin{pmatrix} \mathbf{x}_s^\pm \\ -e^{\frac{i\mu}{2}} \mathbf{x}_s^\pm \end{pmatrix} \in \mathbb{C}^4.$$

Moreover,  $\mathbf{x}_c^\pm$  and  $\mathbf{x}_s^\pm \in \mathbb{C}^2$  are explicitly given as follows:

(1) If  $m_{12}(\lambda) \neq 0$ , then

$$\mathbf{x}_c^\pm = \begin{pmatrix} m_{12}(\lambda)(1 - e^{-\frac{i\mu}{2}}) \\ \rho_c^\pm - m_{11}(\lambda)(1 - e^{-\frac{i\mu}{2}}) \end{pmatrix}, \quad \mathbf{x}_s^\pm = \begin{pmatrix} m_{12}(\lambda)(1 + e^{-\frac{i\mu}{2}}) \\ \rho_s^\pm - m_{11}(\lambda)(1 + e^{-\frac{i\mu}{2}}) \end{pmatrix}.$$

(2) Assume that  $m_{12}(\lambda) = 0$ . Then,

$$\mathbf{x}_c^+ = \begin{pmatrix} \varphi_1 \{\rho_c^+ + (1 + e^{\frac{i\mu}{2}})\} \\ -\{2\Delta m_{11}(e^{-\frac{i\mu}{2}} - 1) + \theta_1(e^{\frac{i\mu}{2}} + 1)\} \end{pmatrix}, \quad \mathbf{x}_c^- = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

(a) If  $0 < |\mu| < \frac{2}{3}\pi$ , then

$$\mathbf{x}_s^- = \begin{pmatrix} \varphi_1 \{\rho_s^- + (1 - e^{\frac{i\mu}{2}})\} \\ -\{-2\Delta m_{11}(1 + e^{-\frac{i\mu}{2}}) + \theta_1(1 - e^{\frac{i\mu}{2}})\} \end{pmatrix}, \quad \mathbf{x}_s^+ = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

(b) If  $\frac{2}{3}\pi < |\mu| \leq \pi$ , then

$$\mathbf{x}_s^+ = \begin{pmatrix} \varphi_1 \{\rho_s^+ + (1 - e^{\frac{i\mu}{2}})\} \\ -\{-2\Delta m_{11}(1 + e^{-\frac{i\mu}{2}}) + \theta_1(1 - e^{\frac{i\mu}{2}})\} \end{pmatrix}, \quad \mathbf{x}_s^- = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

*Proof.* First, we show that there exists some  $\mathbf{x}_c^\pm, \mathbf{x}_s^\pm \in \mathbb{C}^2$  such that  $V(\rho_c^\pm) = \langle \mathbf{w}_c^\pm \rangle$  and  $V(\rho_s^\pm) = \langle \mathbf{w}_s^\pm \rangle$ , where  $\mathbf{w}_c^\pm = \left( \mathbf{x}_c^\pm e^{\frac{i\mu}{2}} \mathbf{x}_c^\pm \right)^\top$ ,  $\mathbf{w}_s^\pm = \left( \mathbf{x}_s^\pm - e^{\frac{i\mu}{2}} \mathbf{x}_s^\pm \right)^\top$ . For  $\rho \in \mathbb{C}$ , we consider the linear equation

$$(\rho E_4 - M(\lambda)) \begin{pmatrix} \mathbf{x} \\ \mathbf{y} \end{pmatrix} = \mathbf{0}, \quad \mathbf{x}, \mathbf{y} \in \mathbb{C}^2.$$

Taking the block form of  $M(\lambda)$  as in Lemma 2.1 into account, we derive

$$(\rho E_2 - A)\mathbf{x} - e^{-i\mu} B\mathbf{y} = \mathbf{0}, \quad (2.8)$$

$$-B\mathbf{x} + (\rho E_2 - A)\mathbf{y} = \mathbf{0}. \quad (2.9)$$

Since the components of  $B$  are explicitly written in Lemma 2.1, we have

$$\det B = \frac{e^{i\mu}}{e^{-i\mu} - 1} \neq 0.$$

Thus, the relationship

$$\mathbf{y} = e^{i\mu} B^{-1}(\rho E_2 - A)\mathbf{x} \quad (2.10)$$

has been established by (2.8). Substituting this into (2.9), we have

$$[\{e^{\frac{i\mu}{2}} B^{-1}(\rho E_2 - A)\}^2 - E_2]\mathbf{x} = \mathbf{0}.$$

This yields

$$\{(e^{-\frac{i\mu}{2}} B)^{-1}(\rho E_2 - A) - E_2\} \{(e^{-\frac{i\mu}{2}} B)^{-1}(\rho E_2 - A) + E_2\} \mathbf{x} = \mathbf{0}, \quad (2.11)$$

$$\{(e^{-\frac{i\mu}{2}} B)^{-1}(\rho E_2 - A) + E_2\} \{(e^{-\frac{i\mu}{2}} B)^{-1}(\rho E_2 - A) - E_2\} \mathbf{x} = \mathbf{0}. \quad (2.12)$$

Let us recall from the proof of Lemma 2.2 that

- $\rho_c^\pm$  are solutions to  $\det(\rho E_2 - A - e^{-\frac{i\mu}{2}} B) = 0$ , and
- $\rho_s^\pm$  are solutions to  $\det(\rho E_2 - A + e^{-\frac{i\mu}{2}} B) = 0$ .

Let us discuss  $\mathbf{x}$  for  $\rho = \rho_c^\pm$ , respectively. By (2.12), we have

$$\{(e^{-\frac{i\mu}{2}} B)^{-1}(\rho_c^\pm E_2 - A) + E_2\} \{(e^{-\frac{i\mu}{2}} B)^{-1}(\rho_c^\pm E_2 - A) - E_2\} \mathbf{x} = \mathbf{0}. \quad (2.13)$$

Due to  $S = \emptyset$ , we have  $\det(\rho_c^\pm E - A + e^{-\frac{i\mu}{2}} B) \neq 0$ . Multiplying (2.13) by  $e^{-\frac{i\mu}{2}} B(\rho_c^\pm E - A + e^{-\frac{i\mu}{2}} B)^{-1} e^{-\frac{i\mu}{2}} B$  from the left, we have

$$(\rho_c^\pm E_2 - A - e^{-\frac{i\mu}{2}} B)\mathbf{x} = \mathbf{0}. \quad (2.14)$$

Let  $\mathbf{x}_c^\pm \in \mathbb{C}^2$  be an eigenvector of  $A + e^{-\frac{i\mu}{2}} B$ . Then, we have  $(\rho_c^\pm E_2 - A)\mathbf{x}_c^\pm = e^{-\frac{i\mu}{2}} B\mathbf{x}_c^\pm$ . Thus, we have  $e^{i\mu} B^{-1}(\rho_c^\pm E_2 - A)\mathbf{x}_c^\pm = e^{\frac{i\mu}{2}} \mathbf{x}_c^\pm$ . This combined with (2.10) yields

$V(\rho_c^\pm) = \langle \mathbf{w}_c^\pm \rangle$ . Similarly,  $V(\rho_s^\pm) = \langle \mathbf{w}_s^\pm \rangle$ , where  $\mathbf{x}_s^\pm \in \mathbb{C}^2$  is an eigenvector of  $A - e^{-\frac{i\mu}{2}}B$ . Note that we use (2.11) instead of (2.12). Except this part, the same procedure brings us  $V(\rho_s^\pm) = \langle \mathbf{w}_s^\pm \rangle$ .

Hereafter, we find an explicit formulae of  $\mathbf{x}_c^\pm$  and  $\mathbf{x}_s^\pm$  as in (1) and (2). In order to prove (1), we assume that  $m_{12} \neq 0$ . To find  $\mathbf{x}_c^\pm$ , we consider the solution  $\mathbf{x} := (x_1 \ x_2)^\top \in \mathbb{C}^2$  to (2.14). Due to  $\det(\rho_c^\pm E_2 - A - e^{-\frac{i\mu}{2}}B) = 0$ , it follows by (2.14) that  $\{\rho_c^\pm - m_{11}(1 - e^{-\frac{i\mu}{2}})\}x_1 + m_{12}(-1 + e^{-\frac{i\mu}{2}})x_2 = 0$ . By virtue of  $m_{12} \neq 0$  and  $\mu \in S^1 \setminus \{0\}$ , we have

$$x_2 = \frac{\rho_c^\pm - m_{11}(1 - e^{-\frac{i\mu}{2}})}{m_{12}(1 - e^{-\frac{i\mu}{2}})}x_1$$

and  $\mathbf{x}_c^\pm$  in (1). We also obtain  $\mathbf{x}_s^\pm$  as in (1) by solving  $(\rho_s^\pm E_2 - A + e^{-\frac{i\mu}{2}}B)\mathbf{x} = \mathbf{0}$ .

Next, we shall show (2). So, assume that  $m_{12} = 0$ . Then, it follows by  $\lambda \notin \sigma_D$  that  $\phi_1' + 2\Delta = 0$  and hence  $\theta_1 + 2\phi_1' = 0$ . This is why we have

$$9\Delta^2 - \Delta_-^2 = 9\left(\frac{\theta_1 + \phi_1'}{2}\right)^2 - \left(\frac{\theta_1 - \phi_1'}{2}\right)^2 = \frac{1}{4}\{9(-\phi_1')^2 - (-3\phi_1')^2\} = 0.$$

Owing to this, we have  $d_c(\mu, \lambda) = -1 - 4\cos^2 \frac{\mu}{4}$  and  $D_c(\mu, \lambda) = (1 - 4\cos^2 \frac{\mu}{4})^2$ . It follows by  $|\mu| \leq \pi$  that  $\sqrt{D_c(\mu, \lambda)} = 4\cos^2 \frac{\mu}{4} - 1 (\geq 1)$ . So, we have  $\rho_c^+ = -\frac{e^{\frac{i\mu}{4}}}{2\cos \frac{\mu}{4}}$  and  $\rho_c^- = -2e^{\frac{i\mu}{4}}\cos \frac{\mu}{4}$ . Therefore, we have

$$\rho_c^+ - m_{11}(1 - e^{-\frac{i\mu}{2}}) = \rho_c^- + (1 + e^{\frac{i\mu}{2}}) = 0, \quad \rho_c^+ + (1 + e^{\frac{i\mu}{2}}) \neq 0, \quad \rho_c^- - m_{11}(1 - e^{-\frac{i\mu}{2}}) \neq 0.$$

Since  $(\rho_c^- E_2 - A - e^{-\frac{i\mu}{2}}B)\mathbf{x} = \mathbf{0}$  is equivalent to  $x_1 = 0$ , we have  $\mathbf{x}_c^-$  in (2). We also have  $\mathbf{x}_c^+$  in (2) because  $(\rho_c^+ E_2 - A - e^{-\frac{i\mu}{2}}B)\mathbf{x} = \mathbf{0}$  is equivalent to

$$\frac{2\Delta m_{11}(e^{-\frac{i\mu}{2}} - 1) + \theta_1(e^{\frac{i\mu}{2}} + 1)}{\phi_1}x_1 + \{\rho_c^+ + (1 + e^{\frac{i\mu}{2}})\}x_2 = 0.$$

On the other hand,  $d_s(\mu, \lambda) = -1 - 4\sin^2 \frac{\mu}{4}$  and  $\sqrt{D_s(\mu, \lambda)} = |1 - 4\sin^2 \frac{\mu}{4}|$ .

(a) Assume that  $0 < |\mu| < \frac{2}{3}\pi$ . Then, we have  $\sqrt{D_s(\mu, \lambda)} = 1 - 4\sin^2 \frac{\mu}{4}$ , which yields  $\rho_s^+ = 2ie^{\frac{i\mu}{4}}\sin \frac{\mu}{4}$  and  $\rho_s^- = \frac{ie^{\frac{i\mu}{4}}}{2\sin \frac{\mu}{4}}$ . Therefore, we have

$$\rho_s^+ + 1 - e^{\frac{i\mu}{2}} = \rho_s^- - m_{11}(1 + e^{-\frac{i\mu}{2}}) = 0, \quad \rho_s^+ - m_{11}(1 + e^{-\frac{i\mu}{2}}) \neq 0, \quad \rho_s^- + 1 - e^{\frac{i\mu}{2}} \neq 0.$$

These are why  $(\rho_s^+ - A + e^{-\frac{i\mu}{2}}B)\mathbf{x} = \mathbf{0}$  and  $(\rho_s^- - A + e^{-\frac{i\mu}{2}}B)\mathbf{x} = \mathbf{0}$  yield  $\mathbf{x}_s^\pm$  in (a).

(b) Assume that  $\frac{2}{3}\pi < |\mu| \leq \pi$ . Then, we have  $\rho_s^+ = \frac{ie^{\frac{i\mu}{4}}}{2\sin \frac{\mu}{4}}$  and  $\rho_s^- = 2ie^{\frac{i\mu}{4}}\sin \frac{\mu}{4}$ . Therefore, we obtain

$$\rho_s^+ - m_{11}(1 + e^{-\frac{i\mu}{2}}) = \rho_s^- + 1 - e^{\frac{i\mu}{2}} = 0, \quad \rho_s^+ + 1 - e^{\frac{i\mu}{2}} \neq 0, \quad \rho_s^- - m_{11}(1 + e^{-\frac{i\mu}{2}}) \neq 0.$$

Thus,  $(\rho_s^+ - A + e^{-\frac{i\mu}{2}}B)\mathbf{x} = \mathbf{0}$  and  $(\rho_s^- - A + e^{-\frac{i\mu}{2}}B)\mathbf{x} = \mathbf{0}$  yield  $\mathbf{x}_s^\pm$  in (b).  $\square$



### 3. Fundamental solutions to $H^b(\mu)y = \lambda y$ .

In this section, we consider the equation to  $H^b(\mu)y = \lambda y$ . In the first subsection, we deal with the case of  $\lambda \in \mathbb{R} \setminus \sigma_D$ . In the second subsection, we discuss the case of  $\lambda \in \sigma_D$ .

#### 3.1. Fundamental solutions in the case of $\lambda \in \mathbb{R} \setminus \sigma_D$ .

Throughout this subsection, we consider  $\lambda \in \mathbb{R} \setminus \sigma_D$ . The aim of this subsection is to find fundamental solutions  $p = (p_{n,j})$ ,  $q = (q_{n,j})$  to  $H^b(\mu)y = \lambda y$  as well as the Kirchhoff–Neumann boundary condition and the initial conditions

$$\begin{pmatrix} p_{1,1}(0, \lambda) \\ p'_{1,1}(0, \lambda) \\ p_{1,4}(0, \lambda) \\ p'_{1,4}(0, \lambda) \end{pmatrix} = \mathbf{e}_1 := \begin{pmatrix} \varphi_1 \\ 2\Delta \\ 0 \\ 0 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} q_{1,1}(0, \lambda) \\ q'_{1,1}(0, \lambda) \\ q_{1,4}(0, \lambda) \\ q'_{1,4}(0, \lambda) \end{pmatrix} = \mathbf{e}_2 := \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}, \quad (3.1)$$

respectively. These conditions are chosen in terms of the following lemma.

**LEMMA 3.1.** *Let  $\lambda \in \mathbb{R} \setminus \sigma_D$  and  $\mu \in S^1$ . Then, any solution  $y$  to  $H^b(\mu)y = \lambda y$  as well as the Kirchhoff–Neumann boundary conditions (1.1)–(1.4) and the Dirichlet boundary condition  $y \equiv 0$  on  $\partial\Gamma_0^b$  satisfies  $y'_{0,2}(0, \lambda) = -y'_{0,3}(1, \lambda)$ . Moreover, we have  $y'_{1,1}(0, \lambda) = 2\Delta c_1$  and  $y_{1,1}(0, \lambda) = c_1 \varphi_1$  if  $y$  satisfies  $y'_{0,2}(0, \lambda) = c_1 \in \mathbb{C}$ .*

*Proof.* Pick a  $y$  satisfying (1.1)–(1.4) and the Dirichlet boundary condition, arbitrarily. Then, we have

$$y_{0,2}(x, \lambda) = y_{0,2}(0, \lambda)\theta(x, \lambda) + y'_{0,2}(0, \lambda)\varphi(x, \lambda) = y'_{0,2}(0, \lambda)\varphi(x, \lambda). \quad (3.2)$$

Using the Kirchhoff–Neumann boundary condition at  $A_1$ , we have  $y_{0,3}(0, \lambda) = y_{0,2}(1, \lambda) = y'_{0,2}(0, \lambda)\varphi_1$ . Substituting this into

$$y_{0,3}(x, \lambda) = y_{0,3}(0, \lambda)\theta(x, \lambda) + y'_{0,3}(0, \lambda)\varphi(x, \lambda), \quad (3.3)$$

we have  $y_{0,3}(x, \lambda) = y'_{0,2}(0, \lambda)\varphi_1\theta(x, \lambda) + y'_{0,3}(0, \lambda)\varphi(x, \lambda)$ . It follows by (3.3) that  $0 = y_{0,3}(1, \lambda) = y'_{0,2}(0, \lambda)\varphi_1\theta_1 + y'_{0,3}(0, \lambda)\varphi_1$ . Because of  $\lambda \notin \sigma_D$ , i.e.,  $\varphi_1 \neq 0$ , we have

$$y'_{0,3}(0, \lambda) = -y'_{0,2}(0, \lambda)\theta_1. \quad (3.4)$$

So, we derive  $y'_{0,3}(1, \lambda) = y'_{0,2}(0, \lambda)\varphi_1\theta'_1 + (-y'_{0,2}(0, \lambda)\theta_1)\varphi'_1 = -y'_{0,2}(0, \lambda)$ .

Next, we assume that  $y$  satisfies  $y'_{0,2}(0, \lambda) = c_1$ . Taking the Kirchhoff–Neumann boundary condition at  $A_1$ , we have  $y'_{1,1}(0, \lambda) = y'_{0,2}(1, \lambda) - y'_{0,3}(0, \lambda) = y'_{0,2}(0, \lambda)\varphi'_1 + y'_{0,2}(0, \lambda)\theta_1 = 2\Delta c_1$  because of (3.2) and (3.4). At last, we have  $y_{1,1}(0, \lambda) = y_{0,2}(1, \lambda) = y'_{0,2}(0, \lambda)\varphi_1 = c_1\varphi_1$  by (3.2).  $\square$

It turns out by Lemma 3.1 that  $p$  satisfies the initial conditions  $p_{0,2}(0, \lambda) = 0$ ,  $p'_{0,2}(0, \lambda) = 1$  (as well as  $p_{0,3}(1, \lambda) = 0$  and  $p'_{0,3}(1, \lambda) = -1$ ). For any solution  $y \in \text{dom}(H^b(\mu))$  to  $H^b(\mu)y = \lambda y$ , it follows by Lemma 3.1 that there exist some  $c_1, c_2 \in \mathbb{C}$  such that  $y$  satisfies the initial condition (1.7). Conversely, for any  $c_1, c_2 \in \mathbb{C}$ , a solution  $y$  to  $H^b(\mu)y = \lambda y$  satisfying (1.1)–(1.4) and (1.7) satisfies the Dirichlet boundary condition on  $\partial\Gamma^\flat$ . Thus,  $p$  and  $q$  are fundamental solutions to  $H^b(\mu)y = \lambda y$ . Next, we give an explicit formula to the above fundamental solution  $p$  and  $q$  to  $H^b(\mu)y = \lambda y$ . Since  $\theta(x, \lambda)$  and  $\varphi(x, \lambda)$  are the fundamental solutions to  $-y'' + qy = \lambda y$ , there exist  $\alpha_{n,j,1}, \beta_{n,j,1}, \alpha_{n,j,2}, \beta_{n,j,2} \in \mathbb{C}$  for each  $(n, j) \in \mathcal{Z}_0$  such that

$$p_{n,j} = \alpha_{n,j,1}\theta(x, \lambda) + \beta_{n,j,1}\varphi(x, \lambda) \quad \text{and} \quad q_{n,j} = \alpha_{n,j,2}\theta(x, \lambda) + \beta_{n,j,2}\varphi(x, \lambda). \quad (3.5)$$

The next aim is to determine the coefficients  $\alpha_{n,j,1}, \beta_{n,j,1}, \alpha_{n,j,2}, \beta_{n,j,2}$  explicitly. To this aim, we furthermore introduce  $M_+(\lambda)$  and  $M_-(\lambda)$  defined as follows:

$$\begin{pmatrix} y_{n,2}(0, \lambda) \\ y'_{n,2}(0, \lambda) \\ y_{n,3}(0, \lambda) \\ y'_{n,3}(0, \lambda) \end{pmatrix} = M_+(\lambda) \begin{pmatrix} y_{n,1}(0, \lambda) \\ y'_{n,1}(0, \lambda) \\ y_{n,4}(0, \lambda) \\ y'_{n,4}(0, \lambda) \end{pmatrix},$$

$$\begin{pmatrix} y_{n,5}(0, \lambda) \\ y'_{n,5}(0, \lambda) \\ y_{n,6}(0, \lambda) \\ y'_{n,6}(0, \lambda) \end{pmatrix} = M_-(\lambda) \begin{pmatrix} y_{n,1}(0, \lambda) \\ y'_{n,1}(0, \lambda) \\ y_{n,4}(0, \lambda) \\ y'_{n,4}(0, \lambda) \end{pmatrix}.$$

The components of  $M_+(\lambda)$  and  $M_-(\lambda)$  are explicitly given as follows:

LEMMA 3.2. Assume that  $\lambda \in \mathbb{R} \setminus \sigma_D$  and  $\mu \in S^1$ . Then, we have

$$M_+(\lambda) = \begin{pmatrix} \theta_1 & \varphi_1 & 0 & 0 \\ \frac{m_{11}-\theta_1^2}{\varphi_1} & \frac{m_{12}}{\varphi_1} - \theta_1 & \frac{m_{13}}{\varphi_1} & \frac{m_{14}}{\varphi_1} \\ m_{11} & m_{12} & m_{13} & m_{14} \\ -\frac{\theta_1}{\varphi_1}m_{11} & -\frac{\theta_1}{\varphi_1}m_{12} & \frac{\theta_1}{\varphi_1}(1-m_{13}) & 1 - \frac{\theta_1}{\varphi_1}m_{14} \end{pmatrix}$$

and

$$M_-(\lambda) = \begin{pmatrix} \theta_1 & \varphi_1 & 0 & 0 \\ \frac{m_{31}}{\varphi_1} & \frac{m_{32}}{\varphi_1} & \frac{m_{33}-\theta_1^2}{\varphi_1} & \frac{m_{34}}{\varphi_1} - \theta_1 \\ m_{31} & m_{32} & m_{33} & m_{34} \\ \frac{e^{i\mu}-\theta_1 m_{31}}{\varphi_1} e^{i\mu} - \frac{\theta_1}{\varphi_1}m_{32} & -\frac{\theta_1}{\varphi_1}m_{33} & -\frac{\theta_1}{\varphi_1}m_{34} \end{pmatrix},$$

where the components of  $M(\lambda) = (m_{ij}(\lambda))$  are explicitly given in Lemma 2.1.

*Proof.* The statements can be shown in a similar way to Lemma 2.1.  $\square$

Let  $P_c^\pm$  and  $P_s^\pm$  be the projections to the eigenspace  $V(\rho_c^\pm)$  and  $V(\rho_s^\pm)$  of the eigenvalues  $\rho_c^\pm$  and  $\rho_s^\pm$  of the transfer matrix  $M(\lambda)$ , respectively. Assume that

$\dim V(\rho_c^\pm) = \dim V(\rho_s^\pm) = 1$ . Putting  $\mathbf{e}_{1,c}^\pm = P_c^\pm \mathbf{e}_1$ ,  $\mathbf{e}_{1,s}^\pm = P_s^\pm \mathbf{e}_1$ ,  $\mathbf{e}_{2,c}^\pm = P_c^\pm \mathbf{e}_2$ ,  $\mathbf{e}_{2,s}^\pm = P_s^\pm \mathbf{e}_2$ , we consider the decompositions

$$\mathbf{e}_1 = \mathbf{e}_{1,c}^+ + \mathbf{e}_{1,c}^- + \mathbf{e}_{1,s}^+ + \mathbf{e}_{1,s}^- \quad \text{and} \quad \mathbf{e}_2 = \mathbf{e}_{2,c}^+ + \mathbf{e}_{2,c}^- + \mathbf{e}_{2,s}^+ + \mathbf{e}_{2,s}^-. \quad (3.6)$$

For  $j = 1, 2, 3, 4, 5, 6$ ,  $\ell = 1, 2$  and  $\bullet = s, c$ , we define  $\alpha_{j,\ell,\bullet}^\pm$  and  $\beta_{j,\ell,\bullet}^\pm$  by

$$(\alpha_{1,\ell,\bullet}^\pm, \beta_{1,\ell,\bullet}^\pm, \alpha_{4,\ell,\bullet}^\pm, \beta_{4,\ell,\bullet}^\pm)^\top = \mathbf{e}_{\ell,\bullet}^\pm, \quad (3.7)$$

$$(\alpha_{2,\ell,\bullet}^\pm, \beta_{2,\ell,\bullet}^\pm, \alpha_{3,\ell,\bullet}^\pm, \beta_{3,\ell,\bullet}^\pm)^\top = M_+(\lambda) \mathbf{e}_{\ell,\bullet}^\pm, \quad (3.8)$$

$$(\alpha_{5,\ell,\bullet}^\pm, \beta_{5,\ell,\bullet}^\pm, \alpha_{6,\ell,\bullet}^\pm, \beta_{6,\ell,\bullet}^\pm)^\top = M_-(\lambda) \mathbf{e}_{\ell,\bullet}^\pm. \quad (3.9)$$

Then, we have an explicit formula of the coefficients  $\alpha_{n,j,1}, \beta_{n,j,1}, \alpha_{n,j,2}, \beta_{n,j,2}$  of the fundamental solutions  $p$  and  $q$ :

LEMMA 3.3. *Let  $\lambda \in \mathbb{R} \setminus \sigma_D$  and  $\mu \in S^1 \setminus \{0\}$ . Assume that  $\dim V(\rho_c^\pm) = \dim V(\rho_s^\pm) = 1$ . Then, the fundamental solutions  $p = (p_{n,j})$  and  $q = (q_{n,j})$  to  $H^\flat(\mu)y = \lambda y$  as well as (1.1)–(1.4) and (3.1) are given by (3.5), where*

$$\alpha_{n,j,1} = (\rho_c^+)^{n-1} \alpha_{j,1,c}^+ + (\rho_c^-)^{n-1} \alpha_{j,1,c}^- + (\rho_s^+)^{n-1} \alpha_{j,1,s}^+ + (\rho_s^-)^{n-1} \alpha_{j,1,s}^-, \quad (3.10)$$

$$\beta_{n,j,1} = (\rho_c^+)^{n-1} \beta_{j,1,c}^+ + (\rho_c^-)^{n-1} \beta_{j,1,c}^- + (\rho_s^+)^{n-1} \beta_{j,1,s}^+ + (\rho_s^-)^{n-1} \beta_{j,1,s}^-, \quad (3.11)$$

$$\alpha_{n,j,2} = (\rho_c^+)^{n-1} \alpha_{j,2,c}^+ + (\rho_c^-)^{n-1} \alpha_{j,2,c}^- + (\rho_s^+)^{n-1} \alpha_{j,2,s}^+ + (\rho_s^-)^{n-1} \alpha_{j,2,s}^-, \quad (3.12)$$

$$\beta_{n,j,2} = (\rho_c^+)^{n-1} \beta_{j,2,c}^+ + (\rho_c^-)^{n-1} \beta_{j,2,c}^- + (\rho_s^+)^{n-1} \beta_{j,2,s}^+ + (\rho_s^-)^{n-1} \beta_{j,2,s}^-. \quad (3.13)$$

*Proof.* Let  $y$  be the solution to  $H^\flat(\mu)y = \lambda y$  as well as (1.7) and (1.1)–(1.4). By the definition of the transfer matrix  $M(\lambda)$ , we have

$$\begin{aligned} & (y_{n,1}(0, \lambda) \ y'_{n,1}(0, \lambda) \ y_{n,4}(0, \lambda) \ y'_{n,4}(0, \lambda))^\top \\ &= M^{n-1}(\lambda) (y_{1,1}(0, \lambda) \ y'_{1,1}(0, \lambda) \ y_{1,4}(0, \lambda) \ y'_{1,4}(0, \lambda))^\top \\ &= M^{n-1}(\lambda) (c_1 \mathbf{e}_1 + c_2 \mathbf{e}_2) \\ &= c_1 M^{n-1}(\lambda) (\mathbf{e}_{1,c}^+ + \mathbf{e}_{1,c}^- + \mathbf{e}_{1,s}^+ + \mathbf{e}_{1,s}^-) + c_2 M^{n-1}(\lambda) (\mathbf{e}_{2,c}^+ + \mathbf{e}_{2,c}^- + \mathbf{e}_{2,s}^+ + \mathbf{e}_{2,s}^-) \\ &= (\rho_c^+)^{n-1} (c_1 \mathbf{e}_{1,c}^+ + c_2 \mathbf{e}_{2,c}^+) + (\rho_c^-)^{n-1} (c_1 \mathbf{e}_{1,c}^- + c_2 \mathbf{e}_{2,c}^-) \\ &\quad + (\rho_s^+)^{n-1} (c_1 \mathbf{e}_{1,s}^+ + c_2 \mathbf{e}_{2,s}^+) + (\rho_s^-)^{n-1} (c_1 \mathbf{e}_{1,s}^- + c_2 \mathbf{e}_{2,s}^-). \end{aligned}$$

This combined with (3.7) yield

$$\begin{aligned} y_{n,j}(0, \lambda) &= c_1 \{ (\rho_c^+)^{n-1} \alpha_{j,1,c}^+ + (\rho_c^-)^{n-1} \alpha_{j,1,c}^- + (\rho_s^+)^{n-1} \alpha_{j,1,s}^+ + (\rho_s^-)^{n-1} \alpha_{j,1,s}^- \} \\ &\quad + c_2 \{ (\rho_c^+)^{n-1} \alpha_{j,2,c}^+ + (\rho_c^-)^{n-1} \alpha_{j,2,c}^- + (\rho_s^+)^{n-1} \alpha_{j,2,s}^+ + (\rho_s^-)^{n-1} \alpha_{j,2,s}^- \}, \end{aligned} \quad (3.14)$$

$$\begin{aligned} y'_{n,j}(0, \lambda) &= c_1 \{ (\rho_c^+)^{n-1} \beta_{j,1,c}^+ + (\rho_c^-)^{n-1} \beta_{j,1,c}^- + (\rho_s^+)^{n-1} \beta_{j,1,s}^+ + (\rho_s^-)^{n-1} \beta_{j,1,s}^- \} \\ &\quad + c_2 \{ (\rho_c^+)^{n-1} \beta_{j,2,c}^+ + (\rho_c^-)^{n-1} \beta_{j,2,c}^- + (\rho_s^+)^{n-1} \beta_{j,2,s}^+ + (\rho_s^-)^{n-1} \beta_{j,2,s}^- \} \end{aligned} \quad (3.15)$$

for  $j = 1, 4$ . Recall that  $y_{n,j}(x, \lambda) = p_{n,j}(x, \lambda)$  ( $y_{n,j}(x, \lambda) = q_{n,j}(x, \lambda)$ , respectively) if  $(c_1, c_2) = (1, 0)$  ( $(c_1, c_2) = (0, 1)$ , respectively). Since  $y_{n,j}(x, \lambda) = y_{n,j}(0, \lambda)\theta(x, \lambda) + y'_{n,j}(0, \lambda)\varphi(x, \lambda)$ , (3.10)–(3.13) are valid for  $j = 1, 4$ .

We next deal with the case of  $j = 2, 3$ . Taking the definition of  $M(\lambda)$  and  $M_+(\lambda)$  into account, we have

$$\begin{aligned} & (y_{n,2}(0, \lambda) y'_{n,2}(0, \lambda) y_{n,3}(0, \lambda) y'_{n,3}(0, \lambda))^{\top} \\ &= M_+(\lambda) M^{n-1}(\lambda) (y_{1,1}(0, \lambda) y'_{1,1}(0, \lambda) y_{1,4}(0, \lambda) y'_{1,4}(0, \lambda))^{\top} \\ &= (\rho_c^+)^{n-1} (c_1 M_+(\lambda) \mathbf{e}_{1,c}^+ + c_2 M_+(\lambda) \mathbf{e}_{2,c}^+) + (\rho_c^-)^{n-1} (c_1 M_+(\lambda) \mathbf{e}_{1,c}^- + c_2 M_+(\lambda) \mathbf{e}_{2,c}^-) \\ & \quad + (\rho_s^+)^{n-1} (c_1 M_+(\lambda) \mathbf{e}_{1,s}^+ + c_2 M_+(\lambda) \mathbf{e}_{2,s}^+) + (\rho_s^-)^{n-1} (c_1 M_+(\lambda) \mathbf{e}_{1,s}^- + c_2 M_+(\lambda) \mathbf{e}_{2,s}^-). \end{aligned}$$

Therefore, we see that (3.14) and (3.15) are valid for  $j = 2, 3$ . After all, (3.10)–(3.13) are valid for  $j = 2, 3$ . On the other hand, it follows by using  $M(\lambda)$  and  $M_-(\lambda)$  that (3.10)–(3.13) are valid for  $j = 5, 6$ .

The results in Lemma 3.3 also can be expressed as follows:

**LEMMA 3.4.** Assume that  $\lambda \in \mathbb{R} \setminus \sigma_D$ ,  $\mu \in S^1 \setminus \{0\}$  and  $\dim V(\rho_c^\pm) = \dim V(\rho_s^\pm) = 1$ . Let  $y = (y_{n,j})_{(n,j) \in \mathbb{Z}_0}$  be the solution to  $H^\flat(\mu)y = \lambda y$  as well as (1.7) and (1.1)–(1.4).

(1) For  $n \in \mathbb{N}$  and  $j = 1, 2, 3, 4, 5, 6$ , we have

$$\begin{aligned} y_{n,j}(x, \lambda) &= (\rho_c^+)^{n-1} (c_1 \eta_{j,1,c}^+ + c_2 \eta_{j,2,c}^+) + (\rho_c^-)^{n-1} (c_1 \eta_{j,1,c}^- + c_2 \eta_{j,2,c}^-) \\ & \quad + (\rho_s^+)^{n-1} (c_1 \eta_{j,1,s}^+ + c_2 \eta_{j,2,s}^+) + (\rho_s^-)^{n-1} (c_1 \eta_{j,1,s}^- + c_2 \eta_{j,2,s}^-), \end{aligned}$$

where  $\eta_{j,\ell,\bullet}^\pm = \eta_{j,\ell,\bullet}^\pm(x, \lambda) = \alpha_{j,\ell,\bullet}^\pm \theta(x, \lambda) + \beta_{j,\ell,\bullet}^\pm \varphi(x, \lambda)$  for  $\ell = 1, 2$  and  $\bullet = s, c$ .

(2) The fundamental solutions  $p = (p_{n,j})_{(n,j) \in \mathbb{Z}_0}$  and  $q = (q_{n,j})_{(n,j) \in \mathbb{Z}_0}$  to  $H^\flat(\mu)y = \lambda y$  as well as (3.1) and (1.1)–(1.4) are expressed as

$$\begin{aligned} p_{n,j}(x, \lambda) &= (\rho_c^+)^{n-1} \eta_{j,1,c}^+ + (\rho_c^-)^{n-1} \eta_{j,1,c}^- + (\rho_s^+)^{n-1} \eta_{j,1,s}^+ + (\rho_s^-)^{n-1} \eta_{j,1,s}^-, \\ q_{n,j}(x, \lambda) &= (\rho_c^+)^{n-1} \eta_{j,2,c}^+ + (\rho_c^-)^{n-1} \eta_{j,2,c}^- + (\rho_s^+)^{n-1} \eta_{j,2,s}^+ + (\rho_s^-)^{n-1} \eta_{j,2,s}^-. \end{aligned}$$

These expression will be used in the proof of our main theorems.

### 3.2. Eigenfunctions to $H^\flat(\mu)$ in the case of $\lambda \in \sigma_D$

In this subsection, we construct infinitely many linear independent eigenfunctions  $\{\Psi_m\}_{m \in \mathbb{N}}$  to  $H^\flat(\mu)$  in the case of  $\lambda \in \sigma_D$ . The result here is an analogy constructed by Korotyaev and Lobanov for carbon nanotubes [5].

Put  $c = \varphi'(1, \lambda)$  and  $\eta = 1 - e^{-i\mu} c^4$  for each  $\mu \in S^1$  and  $\lambda \in \sigma_D$ . For each  $m \in \mathbb{N}$ , we define the function  $\Psi_m = (\Psi_m^{(n,j)})$  on  $\Gamma^\flat$  as follows:

(i) If  $\eta = 0$ , then we put  $\Psi_m^{(m,2)}(x, \lambda) = \varphi(x, \lambda)$ ,  $\Psi_m^{(m,3)}(x, \lambda) = c\varphi(x, \lambda)$ ,  $\Psi_m^{(m,5)}(x, \lambda) = c^2\varphi(x, \lambda)$ ,  $\Psi_m^{(m,6)}(x, \lambda) = c^3\varphi(x, \lambda)$  and  $\Psi_m^{(n,j)}(x, \lambda) = 0$  otherwise.

(ii) If  $\eta \neq 0$ , then we put  $\Psi_m^{(m,1)}(x, \lambda) = \eta \varphi(x, \lambda)$ ,  $\Psi_m^{(m,2)}(x, \lambda) = c \varphi(x, \lambda)$ ,  $\Psi_m^{(m,3)}(x, \lambda) = c^2 \varphi(x, \lambda)$ ,  $\Psi_m^{(m,5)}(x, \lambda) = c^3 \varphi(x, \lambda)$ ,  $\Psi_m^{(m,6)}(x, \lambda) = c^4 \varphi(x, \lambda)$ ,  $\Psi_m^{(m-1,2)}(x, \lambda) = -e^{-i\mu} c^3 \varphi(x, \lambda)$ ,  $\Psi_m^{(m-1,3)}(x, \lambda) = -\varphi(x, \lambda)$ ,  $\Psi_m^{(m-1,5)}(x, \lambda) = -c \varphi(x, \lambda)$ ,  $\Psi_m^{(m-1,6)}(x, \lambda) = -c^2 \varphi(x, \lambda)$  and  $\Psi_m^{(n,j)}(x, \lambda) = 0$  otherwise.

**THEOREM 3.5.** *For  $\lambda \in \sigma_D$ ,  $\mu \in S^1$  and  $m \in \mathbb{N}$ , we have  $\Psi_m \in \text{dom}(H^b(\mu))$  and  $H^b(\mu)\Psi_m = \lambda\Psi_m$ . In particular,  $\lambda \in \sigma_D$  is an eigenvalue to  $H^b(\mu)$  with infinite multiplicities and compactly supported eigenfunctions.*

*Proof.* It follows by straightforward calculations that  $\Psi_m$  satisfies (1.1)–(1.4) and the Dirichlet boundary condition on  $\partial\Gamma^b$ . Moreover, it is clear that  $\Psi_m$  solves  $H^b(\mu)y = \lambda y$  for  $\lambda \in \sigma_D$ .  $\square$

#### 4. Proof of Theorems 1.1 and 1.2

In subsection 3.2, Theorem 1.1 (0) has been already proven. Thus, we prove Theorem 1.1 (1)–(4) and 1.2. Let  $y \neq 0$  be the one in Lemma 3.4. Since  $|a + b + c + d|^2 \leq 4(|a|^2 + |b|^2 + |c|^2 + |d|^2)$  for any  $a, b, c, d \in \mathbb{C}$ , we have

$$\begin{aligned} & \|y_{n,j}\|_{L^2(0,1)}^2 \\ & \leq 4|\rho_c^+|^{2(n-1)} \|c_1\eta_{j,1,c}^+ + c_2\eta_{j,2,c}^+\|_{L^2(0,1)}^2 + 4|\rho_c^-|^{2(n-1)} \|c_1\eta_{j,1,c}^- + c_2\eta_{j,2,c}^-\|_{L^2(0,1)}^2 \\ & \quad + 4|\rho_s^+|^{2(n-1)} \|c_1\eta_{j,1,s}^+ + c_2\eta_{j,2,s}^+\|_{L^2(0,1)}^2 + 4|\rho_s^-|^{2(n-1)} \|c_1\eta_{j,1,s}^- + c_2\eta_{j,2,s}^-\|_{L^2(0,1)}^2. \end{aligned} \quad (4.1)$$

*Proof of Theorem 1.1 (1).* For each  $\mu \in S^1 \setminus \{0\}$ , we fix  $\lambda \in D_1$  satisfying  $S = \emptyset$ . It follows by  $D_s(\mu, \lambda) < 0$ ,  $D_c(\mu, \lambda) < 0$  and Lemma 2.2 that  $|\rho_s^\pm| = |\rho_c^\pm| = 1$ . Put  $C(\mu, \lambda, c_1, c_2) = 16 \max\{\|c_1\eta_{j,1,\bullet}^\pm + c_2\eta_{j,2,\bullet}^\pm\|_{L^2(0,1)}^2 \mid j = 1, \dots, 6, \bullet = s, c\} > 0$ . Taking  $y \neq 0$  in Lemma 3.4, we have  $\|y_{n,j}\|_{L^2(0,1)}^2 \leq C(\mu, \lambda, c_1, c_2)$  for any  $n \in \mathbb{N}$  and  $j$  by (4.1). Thus,  $\|y_{n,j}\|$  is uniformly bounded on  $n \in \mathbb{N}$  and  $j$ . Since  $y$  satisfies the sub-exponential growth condition in the Shnol type theorem [1], we have  $D_1 \setminus L_1 \subset \sigma(H^b(\mu))$ , where  $L_1$  is seen in the proof of Lemma 2.3. Since the Lebesgue measure of  $L_1$  is 0, we have  $D_1 \subset \sigma(H^b(\mu))$ .  $\square$

##### 4.1. Proof of Theorem 1.1 (2) and (3)

In the proof of Theorem 1.1 (1), we derived the uniformly boundedness of  $\|y_{n,j}\|_{L^2(0,1)}^2$  due to  $|\rho_s^\pm| = |\rho_c^\pm| = 1$ . Since the part changes in other cases, the proofs of Theorem 1.1 (2)–(4) and 1.2 turn to be more complicated. In this subsection, we shall give the proof of Theorem 1.1 (2) and (3).

**LEMMA 4.1.** *Assume that  $\lambda \in D_2$  and  $\mu \in S^1 \setminus \{0\}$ . Then,  $d_c(\mu, \lambda) < -4 \cos \frac{\mu}{4}$ ,  $|\rho_s^\pm| = 1$ ,  $|\rho_c^-| > 1$ ,  $|\rho_c^+| < 1$  and  $\rho_c^+ \overline{\rho_c^+} = 1$  hold true.*

*Proof.* We first prove  $d_c(\mu, \lambda) < -4\cos\frac{\mu}{4}$ . Since  $D_c(\mu, \lambda) > 0$ , one of  $d_c(\mu, \lambda) > 4\cos\frac{\mu}{4}$  and  $d_c(\mu, \lambda) < -4\cos\frac{\mu}{4}$  holds true. Let us prove the former does not hold true by contradiction. Seeking a contradiction, we assume the former holds true. It follows by  $D_s(\mu, \lambda) < 0$  that

$$-4\left|\sin\frac{\mu}{4}\right| < 9\Delta^2 - \Delta_-^2 - 1 - 4\sin^2\frac{\mu}{4} < 4\left|\sin\frac{\mu}{4}\right|.$$

This together with  $0 < |\mu| \leq \pi$  yields

$$9\Delta^2 - \Delta_-^2 < \left(2\left|\sin\frac{\mu}{4}\right| + 1\right)^2 \leq (\sqrt{2} + 1)^2.$$

On the other hand, it follows by  $d_c(\mu, \lambda) > 4\cos\frac{\mu}{4}$  that

$$9\Delta^2 - \Delta_-^2 > \left(2\cos\frac{\mu}{4} + 1\right)^2 \geq (\sqrt{2} + 1)^2,$$

which is a contradiction. This is why  $d_c(\mu, \lambda) < -4\cos\frac{\mu}{4}$  only holds true.

It turns out by Lemma 2.2 and  $D_s(\mu, \lambda) < 0$  that

$$|\rho_s^\pm| = \frac{\sqrt{d_s^2(\mu, \lambda) + (-D_s(\mu, \lambda))}}{4\left|\sin\frac{\mu}{4}\right|} = \frac{\sqrt{16\sin^2\frac{\mu}{4}}}{4\left|\sin\frac{\mu}{4}\right|} = 1.$$

It follows by  $d_c(\mu, \lambda) < -4\cos\frac{\mu}{4} < 0$  that

$$|\rho_c^-| = \frac{-d_c(\mu, \lambda) + \sqrt{d_c^2(\mu, \lambda) - 16\cos^2\frac{\mu}{4}}}{4\cos\frac{\mu}{4}} > \frac{4\cos\frac{\mu}{4} + 0}{4\cos\frac{\mu}{4}} = 1.$$

This combined with

$$\rho_c^+ \overline{\rho_c^-} = \frac{d_c(\mu, \lambda) + \sqrt{d_c^2(\mu, \lambda)}}{4e^{\frac{-i\mu}{4}} \cos\frac{\mu}{4}} \cdot \frac{d_c(\mu, \lambda) - \sqrt{d_c^2(\mu, \lambda)}}{4e^{\frac{i\mu}{4}} \cos\frac{\mu}{4}} = \frac{16\cos^2\frac{\mu}{4}}{16\cos^2\frac{\mu}{4}} = 1$$

yields  $|\rho_c^+| < 1$ .  $\square$

Although we utilize the Shnol's type theorem in [1] to prove  $D_2 \subset \sigma(H^b(\mu))$  for  $\mu \in S^1 \setminus \{0\}$ , it is not clear due to the results in this lemma ( $|\rho_s^\pm| = 1$ ,  $|\rho_c^-| > 1$ ,  $|\rho_c^+| < 1$ , especially) for that there exist some  $(c_1, c_2) \in \mathbb{C}^2 \setminus \{(0, 0)\}$  satisfying  $\|y_{n,j}\|_{L^2(0,1)}^2$  is uniformly bounded on  $n \in \mathbb{N}$  and  $j = 1, 2, 3, 4, 5, 6$ . The highlight of this paper is the followings:

- We utilize the Cramer's rule to determine  $(c_1, c_2) \in \mathbb{C}^2 \setminus \{(0, 0)\}$  producing a non-trivial  $y$  which has uniformly bounded norm  $\|y_{n,j}\|_{L(0,1)}$  on  $(n, j)$  and solves  $H^b(\mu)y = \lambda y$  as well as (1.1)–(1.4) and (1.7).

Recall (3.6), Lemma 2.3 and 2.4. Then, there exist the coefficients  $\gamma_c^+$ ,  $\gamma_c^-$ ,  $\gamma_s^+$ ,  $\gamma_s^-$ ,  $\delta_c^+$ ,  $\delta_c^-$ ,  $\delta_s^+$ ,  $\delta_s^- \in \mathbb{C}$  of the eigenfunction expansions

$$\mathbf{e}_1 = \mathbf{e}_{1,c}^+ + \mathbf{e}_{1,c}^- + \mathbf{e}_{1,s}^+ + \mathbf{e}_{1,s}^- = \gamma_c^+ \mathbf{w}_c^+ + \gamma_c^- \mathbf{w}_c^- + \gamma_s^+ \mathbf{w}_s^+ + \gamma_s^- \mathbf{w}_s^-, \quad (4.2)$$

$$\mathbf{e}_2 = \mathbf{e}_{2,c}^+ + \mathbf{e}_{2,c}^- + \mathbf{e}_{2,s}^+ + \mathbf{e}_{2,s}^- = \delta_c^+ \mathbf{w}_c^+ + \delta_c^- \mathbf{w}_c^- + \delta_s^+ \mathbf{w}_s^+ + \delta_s^- \mathbf{w}_s^-. \quad (4.3)$$

LEMMA 4.2. Assume that  $\lambda \in D_2$  and  $\mu \in S^1 \setminus \{0\}$ . Then, we have  $\gamma_c^- \neq 0$  and  $\delta_c^- \neq 0$  in the eigenfunction expansion (4.2) and (4.3).

In order to make our discussion clear, we shall show Theorem 1.1 (2) using Lemma 4.2 before the proof of the lemma.

*Proof of Theorem 1.1 (2).* Fix  $\lambda \in D_2$  and  $\mu \in S^1 \setminus \{0\}$ . It follows by  $\mathbf{e}_{1,c}^- = \gamma_c^- \mathbf{w}_c^-$  and  $\mathbf{e}_{2,c}^- = \delta_c^- \mathbf{w}_c^-$  that  $\delta_c^- \mathbf{e}_{1,c}^- + (-\gamma_c^-) \mathbf{e}_{2,c}^- = \mathbf{0}$ . This combined with (3.7)–(3.9) give us the relationship

$$\delta_c^- \alpha_{j,1,c}^- + (-\gamma_c^-) \alpha_{j,2,c}^- = 0 \quad \text{and} \quad \delta_c^- \beta_{j,1,c}^- + (-\gamma_c^-) \beta_{j,2,c}^- = 0$$

for any  $j = 1, 2, 3, 4, 5, 6$ . Therefore, we have

$$\delta_c^- \eta_{j,1,c}^-(x, \lambda) + (-\gamma_c^-) \eta_{j,2,c}^-(x, \lambda) = 0$$

for all  $j = 1, 2, 3, 4, 5, 6$  because  $\eta_{j,\ell,\bullet}^\pm(x, \lambda) = \alpha_{j,\ell,\bullet}^\pm \theta(x, \lambda) + \beta_{j,\ell,\bullet}^\pm \varphi(x, \lambda)$  (which is defined in Lemma 3.4). Thus, it turns out by (4.1) that

$$\begin{aligned} & \|y_{n,j}\|_{L^2(0,1)}^2 \\ & \leq 4|\rho_c^+|^{2(n-1)} \|\delta_c^- \eta_{j,1,c}^+ - \gamma_c^- \eta_{j,2,c}^+\|_{L^2(0,1)}^2 + 4|\rho_s^+|^{2(n-1)} \|\delta_c^- \eta_{j,1,s}^+ - \gamma_c^- \eta_{j,2,s}^+\|_{L^2(0,1)}^2 \\ & \quad + 4|\rho_s^-|^{2(n-1)} \|\delta_c^- \eta_{j,1,s}^- - \gamma_c^- \eta_{j,2,s}^-\|_{L^2(0,1)}^2 \end{aligned}$$

for any  $n \in \mathbb{N}$  and  $j = 1, 2, 3, 4, 5, 6$ . According to Lemma 4.1, we have  $|\rho_s^\pm| = 1$ ,  $|\rho_c^-| > 1$ ,  $|\rho_c^+| < 1$ . So, this  $\|y_{n,j}\|_{L^2(0,1)}$  is uniformly bounded on  $n \in \mathbb{N}$  and  $j = 1, 2, 3, 4, 5, 6$ . Note that our  $y$  is the solution to  $H^b(\mu)y = \lambda y$  as well as (1.1)–(1.4) and the Dirichlet boundary condition

$$(y_{1,1}(0, \lambda) \ y'_{1,1}(0, \lambda) \ y_{1,4}(0, \lambda) \ y'_{1,4}(0, \lambda))^T = \delta_c^- \mathbf{e}_1 + (-\gamma_c^-) \mathbf{e}_2.$$

By virtue of  $\gamma_c^- \neq 0$  and  $\delta_c^- \neq 0$ , this  $y$  is non-trivial. The existence of such  $y$  yields the sub-exponential condition in the Shnol's theorem [1].  $\square$

As seen in the proof of Theorem 1.1 (2), Lemma 4.2 plays the role to tune the volumes of channels  $(c_1, c_2) \in \mathbb{C}^2 \setminus \{(0, 0)\}$  to make a non-trivial wave  $y$  satisfying the sub-exponentially growth condition. In order to finish the proof of Theorem 1.1 (2), we need to prove Lemma 4.2. To prove  $\gamma_c^- \neq 0$ , we consider the linear equation (4.2) whose the argumented coefficient matrix  $(\mathbf{w}_c^+ \ \mathbf{w}_c^- \ \mathbf{w}_s^+ \ \mathbf{w}_s^- \mid \mathbf{e}_1)$ . Although all vectors  $\mathbf{w}_c^+$ ,  $\mathbf{w}_c^-$ ,  $\mathbf{w}_s^+$ ,  $\mathbf{w}_s^-$ ,  $\mathbf{e}_1$  are explicitly given in Lemma 2.4 and (3.1), elementary

row operations of the matrix seem to be not practical. However, it is enough to find  $\gamma_c^- \neq 0$  in order to find our desired wave. Thus, *the Cramer's rule* can be an effective tool. Introduce new notations

$$\mathbf{e}_1^+ = \begin{pmatrix} \varphi_1 \\ 2\Delta \end{pmatrix} \quad \text{and} \quad \mathbf{e}_2^- = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \quad (4.4)$$

*Proof of Lemma 4.2.* We show  $\gamma_c^- \neq 0$ . It follows from Lemma 2.3 that all eigenvalues  $\rho_s^+, \rho_s^-, \rho_c^+, \rho_c^-$  are distinct. Thus,  $\mathbf{w}_c^+, \mathbf{w}_c^-, \mathbf{w}_s^+, \mathbf{w}_s^-$  are linearly independent. Applying the Cramer's rule, we have

$$\gamma_c^- = \frac{\det(\mathbf{w}_c^+ \mathbf{e}_1 \mathbf{w}_s^+ \mathbf{w}_s^-)}{\det(\mathbf{w}_c^+ \mathbf{w}_c^- \mathbf{w}_s^+ \mathbf{w}_s^-)}.$$

In order to prove  $\gamma_c^- \neq 0$ , it suffices to show that  $\det(\mathbf{w}_c^+ \mathbf{e}_1 \mathbf{w}_s^+ \mathbf{w}_s^-) \neq 0$ . It follows by Lemma 2.4 that

$$\det(\mathbf{w}_c^+ \mathbf{e}_1 \mathbf{w}_s^+ \mathbf{w}_s^-) = \begin{vmatrix} \mathbf{x}_c^+ & \mathbf{e}_1^+ & \mathbf{x}_s^+ & \mathbf{x}_s^- \\ e^{\frac{i\mu}{2}} \mathbf{x}_c^+ & \mathbf{0} & -e^{\frac{i\mu}{2}} \mathbf{x}_s^+ & -e^{\frac{i\mu}{2}} \mathbf{x}_s^- \end{vmatrix} = \begin{vmatrix} \mathbf{x}_c^+ & \mathbf{e}_1^+ & \mathbf{x}_s^+ & \mathbf{x}_s^- \\ 2e^{\frac{i\mu}{2}} \mathbf{x}_c^+ & e^{\frac{i\mu}{2}} \mathbf{e}_1^+ & \mathbf{0} & \mathbf{0} \end{vmatrix}.$$

Since  $\begin{vmatrix} A_{11} & A_{12} \\ A_{21} & O \end{vmatrix} = |A_{12}| |A_{21}|$  holds true for any  $2 \times 2$  matrices  $A_{11}, A_{12}, A_{21}$  and the  $2 \times 2$  zero matrix  $O$ , we have

$$\tilde{\gamma}_c^- := \det(\mathbf{w}_c^+ \mathbf{e}_1 \mathbf{w}_s^+ \mathbf{w}_s^-) = 2e^{i\mu} |\mathbf{x}_s^+ \mathbf{x}_s^-| \times |\mathbf{x}_c^+ \mathbf{e}_1^+|. \quad (4.5)$$

Since  $\mathbf{w}_s^+$  and  $\mathbf{w}_s^-$  are linearly independent, so  $\mathbf{x}_s^+$  and  $\mathbf{x}_s^-$  are. So,  $|\mathbf{x}_s^+ \mathbf{x}_s^-| \neq 0$ . Let us show  $|\mathbf{x}_c^+ \mathbf{e}_1^+| \neq 0$  by straightforward calculations. We claim that  $m_{12} \neq 0$ . Seeking a contradiction, we assume that  $m_{12} = 0$ . This yield  $2\Delta + \varphi_1' = 0$  and  $9\Delta^2 - \Delta^2 = 0$ . So, we have  $d_s(\mu, \lambda) = -1 - 4\sin^2 \frac{\mu}{4}$  and  $D_s(\mu, \lambda) = (-1 - 4\sin^2 \frac{\mu}{4})^2 - 16\sin^2 \frac{\mu}{4} = (4\sin^2 \frac{\mu}{4} - 1)^2 \geq 0$ , which contradicts  $\lambda \in D_2$ . Thus, we use Lemma 2.4 (1). Substituting  $m_{11}$  and  $m_{12}$  obtained in Lemma 2.1 into  $\mathbf{x}_c^+$  obtained in Lemma 2.4 (1), we have

$$|\mathbf{x}_c^+ \mathbf{e}_1^+| = \varphi_1 \left( \frac{8\Delta^2 + \theta_1' \varphi_1}{1 + e^{-\frac{i\mu}{2}}} - \rho_c^+ \right).$$

Substituting  $1 + e^{-\frac{i\mu}{2}} = 2e^{-\frac{i\mu}{4}} \cos \frac{\mu}{4}$  and  $8\Delta^2 + \theta_1' \varphi_1 = 9\Delta^2 - \Delta_-^2 - 1$  here and then using Lemma 2.2, we have

$$|\mathbf{x}_c^+ \mathbf{e}_1^+| = \frac{\varphi_1}{4e^{-\frac{i\mu}{4}} \cos \frac{\mu}{4}} \left( d_c - \sqrt{D_c} + 8\cos^2 \frac{\mu}{4} \right). \quad (4.6)$$

Seeking a contradiction, we assume  $d_c - \sqrt{D_c} + 8\cos^2 \frac{\mu}{4} = 0$ . Squaring  $d_c + 8\cos^2 \frac{\mu}{4} = \sqrt{D_c}$ , we have  $d_c = -1 - 4\cos^2 \frac{\mu}{4}$  and  $9\Delta^2 - \Delta_-^2 = 0$ . The latter contradicts  $\lambda \in D_2$ . As a result, we have  $d_c - \sqrt{D_c} + 8\cos^2 \frac{\mu}{4} \neq 0$ . This combined with  $\lambda \notin \sigma_D$  and (4.6) yield  $|\mathbf{x}_c^+ \mathbf{e}_1^+| \neq 0$ . So, we have  $\gamma_c^- \neq 0$ .



Secondly, we prove  $\delta_c^- \neq 0$ . In a similar way, we have

$$\det(\mathbf{w}_c^+ \mathbf{e}_2 \mathbf{w}_s^+ \mathbf{w}_s^-) = 2e^{\frac{i\mu}{2}} |\mathbf{x}_s^+ \mathbf{x}_s^-| \times m_{12}(1 - e^{-\frac{i\mu}{2}}).$$

Note that  $|\mathbf{x}_s^+ \mathbf{x}_s^-| \neq 0$  by the linearly independence of  $\mathbf{w}_s^+$  and  $\mathbf{w}_s^-$ . Furthermore,  $m_{12} \neq 0$  has already been proven. Thus, we have  $\delta_c^- \neq 0$ .  $\square$

Here, the proof of Theorem 1.1 (2) has been completed. The proof of Theorem 1.1 (3) can be shown in a similar way to Theorem 1.1 (2). We set materials for the proof of Theorem 1.1 (3) without their proofs.

**LEMMA 4.3.** Assume that  $\lambda \in D_3$  and  $\mu \in S^1 \setminus \{0, \pm \frac{2}{3}\pi\}$ . Then,  $d_s(\mu, \lambda) > 4|\sin \frac{\mu}{4}|$ ,  $|\rho_c^\pm| = 1$ ,  $|\rho_s^+| > 1$ ,  $|\rho_s^-| < 1$  and  $\rho_s^+ \overline{\rho_s^-} = 1$  hold true.

The proof of this lemma has done in a similar way to Lemma 4.1. The reason why we need the assumption  $\mu \neq \pm \frac{2}{3}\pi$  is due to Lemma 2.3. Namely, we have distinct 4 eigenvalues  $\rho_s^\pm, \rho_c^\pm$  in the additional assumption.

**LEMMA 4.4.** Assume that  $\lambda \in D_3$  and  $\mu \in S^1 \setminus \{0, \pm \frac{2}{3}\pi\}$ . Then, we have  $\gamma_s^+ \neq$  and  $\delta_s^+ \neq 0$  in the eigenfunction expansions (4.2) and (4.3).

The proof of this lemma has done in a similar way to Lemma 4.2. For readers' sake, we only record the followings:

$$\det(\mathbf{w}_c^+ \mathbf{w}_c^- \mathbf{e}_1 \mathbf{w}_s^-) = 2e^{i\mu} |\mathbf{x}_c^+ \mathbf{x}_c^-| \times \frac{-\varphi_1}{4ie^{-\frac{i\mu}{4}} \sin \frac{\mu}{4}} \left( d_s + \sqrt{D_s} + 8 \sin^2 \frac{\mu}{4} \right) \neq 0.$$

$$\det(\mathbf{w}_c^+ \mathbf{w}_c^- \mathbf{e}_2 \mathbf{w}_s^-) = 2e^{\frac{i\mu}{2}} |\mathbf{x}_c^+ \mathbf{x}_c^-| \times m_{12}(1 + e^{-\frac{i\mu}{2}}) \neq 0.$$

*Proof of Theorem 1.1 (3).* Considering the solution  $y$  to  $H^b y = \lambda y$  as well as (1.1)–(1.2) and

$$(y_{1,1}(0, \lambda) y'_{1,1}(0, \lambda) y_{1,4}(0, \lambda) y'_{1,4}(0, \lambda))^T = \delta_s^+ \mathbf{e}_1 + (-\gamma_s^+) \mathbf{e}_2$$

and taking into account Lemma 4.3 and 4.4, we obtain a non-trivial solution satisfying the sub-exponential growth condition in [1]. The detail is similar to the proof of Theorem 1.1 (2).  $\square$

## 4.2. Proof of Theorem 1.1 (4) and 1.2.

In the last subsection, we deal with the case of  $\lambda \in D_4$  and  $\mu \in S^1 \setminus \{0\}$ . The following cases do not happen:

- the case of  $d_c(\mu, \lambda) > 4 \cos \frac{\mu}{4}$  and  $d_s(\mu, \lambda) < -4 |\sin \frac{\mu}{4}|$ .
- the case of  $d_c(\mu, \lambda) < -4 \cos \frac{\mu}{4}$  and  $d_s(\mu, \lambda) > 4 |\sin \frac{\mu}{4}|$ .

So, we have  $D_4 = D_4^+ \cup D_4^-$ . To begin with, we explain the reason why we split the subsections.

LEMMA 4.5. Assume that  $\mu \in S^1 \setminus \{0\}$ .

(i) If  $\lambda \in D_4^+$ , then  $\rho_s^+ \overline{\rho_s^-} = \rho_c^+ \overline{\rho_c^-} = 1$ ,  $|\rho_s^+| > 1$ ,  $|\rho_c^+| > 1$ ,  $|\rho_s^-| < 1$ ,  $|\rho_c^-| < 1$ .

(ii) If  $\lambda \in D_4^-$ , then  $\rho_s^+ \overline{\rho_s^-} = \rho_c^+ \overline{\rho_c^-} = 1$ ,  $|\rho_s^+| < 1$ ,  $|\rho_c^+| < 1$ ,  $|\rho_s^-| > 1$ ,  $|\rho_c^-| > 1$ .

These results can be shown in a similar way to Lemmas 4.1 and 4.3. From the point of view of Lemma 4.5, there are 2 terms in (4.1) which might grow exponentially. The possibilities yield the difference between this and the previous subsections. Since the proof of Theorem 1.1 (4) is relatively easy to deal with, we discuss it first.

LEMMA 4.6. Assume that  $\lambda \in D_4^+$  and  $\mu \in S^1 \setminus \{0\}$ . Then, we have  $\gamma_c^+ \neq 0$ ,  $\gamma_s^+ \neq 0$ ,  $\delta_c^+ \neq 0$  and  $\delta_s^+ \neq 0$  in the eigenfunction expansions (4.2) and (4.3).

*Proof.* Unlike the case of  $\lambda \in D_4^-$  (see Lemma 4.11 below), we cannot fail to have  $m_{12} \neq 0$  if  $\lambda \in D_4^+$ . To make sure it, we assume that  $m_{12} = 0$  seeking a contradiction. Then, we have  $2\Delta + \phi_1'$  and hence  $9\Delta^2 - \Delta_-^2 = 0$ . Substituting this into  $d_c(\mu, \lambda) > 4 \cos \frac{\mu}{4}$ , we have  $0 = 9\Delta^2 - \Delta_-^2 > (2 \cos \frac{\mu}{4} + 1)^2 \geq (\sqrt{2} + 1)^2$ . So, we have  $m_{12} \neq 0$ . In a similar manner to Lemma 4.2, we have

$$\tilde{\gamma}_s^+ := \det(\mathbf{w}_c^+ \mathbf{w}_c^- \mathbf{e}_1 \mathbf{w}_s^-) = -\frac{e^{i\mu} \varphi_1 |\mathbf{x}_c^+ \mathbf{x}_c^-|}{2ie^{-\frac{i\mu}{4}} \sin \frac{\mu}{4}} \left( d_s + \sqrt{D_s} + 8 \sin^2 \frac{\mu}{4} \right), \quad (4.7)$$

$$\tilde{\gamma}_c^+ := \det(\mathbf{e}_1 \mathbf{w}_c^- \mathbf{w}_s^+ \mathbf{w}_s^-) = -\frac{e^{i\mu} \varphi_1 |\mathbf{x}_s^+ \mathbf{x}_s^-|}{2e^{-\frac{i\mu}{4}} \cos \frac{\mu}{4}} \left( d_c + \sqrt{D_c} + 8 \cos^2 \frac{\mu}{4} \right), \quad (4.8)$$

$$\tilde{\delta}_s^+ := \det(\mathbf{w}_c^+ \mathbf{w}_c^- \mathbf{e}_2 \mathbf{w}_s^-) = 2e^{\frac{i\mu}{2}} |\mathbf{x}_c^+ \mathbf{x}_c^-| (e^{-\frac{i\mu}{2}} + 1) m_{12} \neq 0, \quad (4.9)$$

$$\tilde{\delta}_c^+ := \det(\mathbf{e}_2 \mathbf{w}_c^- \mathbf{w}_s^+ \mathbf{w}_s^-) = 2e^{\frac{i\mu}{2}} |\mathbf{x}_s^+ \mathbf{x}_s^-| (e^{-\frac{i\mu}{2}} - 1) m_{12} \neq 0. \quad (4.10)$$

We claim that  $d_s + \sqrt{D_s} + 8 \sin^2 \frac{\mu}{4} \neq 0$  and  $d_c + \sqrt{D_c} + 8 \cos^2 \frac{\mu}{4} \neq 0$ . In fact, we have  $9\Delta^2 - \Delta_-^2 = 0$  in both cases of  $d_s + \sqrt{D_s} + 8 \sin^2 \frac{\mu}{4} = 0$  and  $d_c + \sqrt{D_c} + 8 \cos^2 \frac{\mu}{4} = 0$ . We reuse the fact that  $9\Delta^2 - \Delta_-^2 = 0$  contradicts  $d_c > 4 \cos \frac{\mu}{4}$ .

So, we have  $\det(\mathbf{w}_c^+ \mathbf{w}_c^- \mathbf{e}_1 \mathbf{w}_s^-) \neq 0$  and  $\det(\mathbf{e}_1 \mathbf{w}_c^- \mathbf{w}_s^+ \mathbf{w}_s^-) \neq 0$ . It turns out by the Cramer's rule that  $\gamma_c^+ \neq 0$ ,  $\gamma_s^+ \neq 0$ ,  $\delta_c^+ \neq 0$  and  $\delta_s^+ \neq 0$ .  $\square$

Next, we are interested in whether or not we can find  $(c_1, c_2) \in \mathbb{C}^2 \setminus \{(0, 0)\}$  satisfying  $c_1 \eta_{j,1,c}^+ + c_2 \eta_{j,2,c}^+ = c_1 \eta_{j,1,s}^+ + c_2 \eta_{j,2,s}^+ = 0$  for all  $j = 1, 2, 3, 4, 5, 6$  from the point of (4.1).

LEMMA 4.7. Let  $\lambda \in D_4^+$  and  $\mu \in S^1 \setminus \{0, \pm\pi\}$ . Then, we have  $\delta_c^+ \gamma_s^+ - \gamma_c^+ \delta_s^+ \neq 0$ .

*Proof.* Recall the notations  $\tilde{\gamma}_s^+, \tilde{\gamma}_c^+, \tilde{\delta}_s^+, \tilde{\delta}_c^+$  from (4.7)–(4.10). Since Lemma 2.3 (4) means  $\det(\mathbf{w}_c^+ \mathbf{w}_c^- \mathbf{w}_s^+ \mathbf{w}_s^-) \neq 0$ , it suffices to show that  $-\tilde{\delta}_c^+ \tilde{\gamma}_s^+ + \tilde{\delta}_s^+ \tilde{\gamma}_c^+ \neq 0$ . Using  $1 + e^{-\frac{i\mu}{2}} = 2e^{-\frac{i\mu}{4}} \cos \frac{\mu}{4}$  and  $1 - e^{-\frac{i\mu}{2}} = 2ie^{-\frac{i\mu}{4}} \sin \frac{\mu}{4}$ , we have

$$-\tilde{\delta}_c^+ \tilde{\gamma}_s^+ + \tilde{\delta}_s^+ \tilde{\gamma}_c^+ = 2e^{\frac{3i\mu}{2}} m_{12} \varphi_1 \left| \mathbf{x}_s^+ \mathbf{x}_s^- \right| \left| \mathbf{x}_c^+ \mathbf{x}_c^- \right| (-d_s - \sqrt{D_s} - d_c - \sqrt{D_c} - 8).$$

Since  $d_c(\mu, \lambda) > 4 \cos \frac{\mu}{4}$ ,  $d_s(\mu, \lambda) > 4 \left| \sin \frac{\mu}{4} \right|$ ,  $D_s(\mu, \lambda) > 0$  and  $D_c(\mu, \lambda) > 0$ , we have

$$-d_s - \sqrt{D_s} - d_c - \sqrt{D_c} - 8 < 0.$$

Moreover, we derived  $m_{12}(\lambda) \neq 0$  in Lemma 4.6. Thus, we have  $\delta_c^+ \gamma_s^+ - \gamma_c^+ \delta_s^+ \neq 0$ .  $\square$

LEMMA 4.8. *Let  $\lambda \in D_4^+$  and  $\mu \in S^1 \setminus \{0, \pm\pi\}$ . Then, there is no pair  $(c_1, c_2) \in \mathbb{C}^2 \setminus \{(0, 0)\}$  satisfying  $c_1 \eta_{j,1,c}^+ + c_2 \eta_{j,2,c}^+ = c_1 \eta_{j,1,s}^+ + c_2 \eta_{j,2,s}^+ = 0$  for all  $j = 1, 2, 3, 4, 5, 6$ .*

*Proof.* It follows that  $\mathbf{e}_{1,s}^+ = \frac{\gamma_c^+}{\delta_s^+} \mathbf{e}_{2,s}^+$  and  $\mathbf{e}_{1,c}^+ = \frac{\gamma_c^+}{\delta_c^+} \mathbf{e}_{2,c}^+$  by  $\mathbf{e}_{1,2}^+ = \gamma_s^+ \mathbf{w}_s^+$ ,  $\mathbf{e}_{2,s}^+ = \delta_s^+ \mathbf{w}_s^+$ ,  $\mathbf{e}_{1,c}^+ = \gamma_c^+ \mathbf{w}_c^+$ ,  $\mathbf{e}_{2,c}^+ = \delta_c^+ \mathbf{w}_c^+$ , (4.2), (4.3) and Lemma 4.7. Substituting  $\mathbf{e}_{1,s}^+ = \frac{\gamma_c^+}{\delta_s^+} \mathbf{e}_{2,s}^+$  and  $\mathbf{e}_{1,c}^+ = \frac{\gamma_c^+}{\delta_c^+} \mathbf{e}_{2,c}^+$  into (3.7)–(3.9), we have

$$\begin{aligned} \alpha_{j,1,\bullet}^+ &= \frac{\gamma_c^+}{\delta_s^+} \alpha_{j,2,\bullet}^+, \quad \beta_{j,1,\bullet}^+ = \frac{\gamma_c^+}{\delta_c^+} \beta_{j,2,\bullet}^+, \\ \eta_{j,1,\bullet}^+ &= \alpha_{j,1,\bullet}^+ \theta(x, \lambda) + \beta_{j,1,\bullet}^+ \varphi(x, \lambda) \\ &= \frac{\gamma_c^+}{\delta_s^+} (\alpha_{j,2,\bullet}^+ \theta(x, \lambda) + \beta_{j,2,\bullet}^+ \varphi(x, \lambda)) \\ &= \frac{\gamma_c^+}{\delta_s^+} \eta_{j,2,\bullet}^+. \end{aligned} \tag{4.11}$$

for  $\bullet = s, c$ . So, we have  $\delta_c^+ \eta_{j,1,c}^+ - \gamma_c^+ \eta_{j,2,c}^+ = \delta_s^+ \eta_{j,1,s}^+ - \gamma_s^+ \eta_{j,2,s}^+ = 0$  for all  $j$ .

Seeking a contradiction, we assume that there is some pair  $(c_1, c_2) \in \mathbb{C}^2 \setminus \{(0, 0)\}$  satisfying  $c_1 \eta_{j,1,c}^+ + c_2 \eta_{j,2,c}^+ = c_1 \eta_{j,1,s}^+ + c_2 \eta_{j,2,s}^+ = 0$  for all  $j = 1, 2, 3, 4, 5, 6$ . Substituting  $\delta_c^+ \eta_{j,1,c}^+ = \gamma_c^+ \eta_{j,2,c}^+$  into  $\delta_c^+ (c_1 \eta_{j,1,c}^+ + c_2 \eta_{j,2,c}^+) = 0$ , we have  $c_1 \gamma_c^+ + c_2 \delta_c^+ = 0$ . Substituting  $\delta_s^+ \eta_{j,1,s}^+ = \gamma_s^+ \eta_{j,2,s}^+$  into  $\delta_s^+ (c_1 \eta_{j,1,s}^+ + c_2 \eta_{j,2,s}^+) = 0$ , we have  $c_1 \gamma_s^+ + c_2 \delta_s^+ = 0$ . It follows by Lemma 4.7 that  $c_1 = c_2 = 0$ . After all, there does not exist such a pair.  $\square$

Taking the result and (4.1) into account, we are wondering if  $\|y_{n,j}\|_{L^2(0,1)}^2$  might not be uniformly bounded on  $n \in \mathbb{N}$  and  $j = 1, 2, 3, 4, 5, 6$ . To make sure it, we prepare the followings:

LEMMA 4.9. *Assume that  $\lambda \in D_4^+$  and  $\mu \in S^1 \setminus \{0, \pm\pi\}$ . For all  $(c_1, c_2) \in \mathbb{C}^2 \setminus \{(0, 0)\}$ , we have  $(c_1 \gamma_c^+ + c_2 \delta_c^+, c_1 \gamma_s^+ + c_2 \delta_s^+) \neq (0, 0)$ .*

*Proof.* In the case of  $c_1 \neq -\frac{\delta_c^+}{\gamma_c^+}c_2$ , it directly means the result. So, we show that  $c_1\gamma_s^+ + c_2\delta_s^+ \neq 0$  if  $c_1 = -\frac{\delta_c^+}{\gamma_c^+}c_2$  and  $c_2 \neq 0$ . Assume that  $c_1 = -\frac{\delta_c^+}{\gamma_c^+}c_2$  and  $c_2 \neq 0$ . Then, our goal is to show that  $-\delta_c^+\gamma_s^+ + \delta_s^+\gamma_c^+ \neq 0$ , which has been already derived in the previous lemma.  $\square$

*Proof of Theorem 1.1 (4).* Substituting (4.11) into the expression in Lemma 3.4 (1), we have

$$\begin{aligned} y_{n,j}(x, \lambda) &= (\rho_c^+)^{n-1} \left( c_1 \frac{\gamma_c^+}{\delta_c^+} + c_2 \right) \eta_{j,2,c}^+ + (\rho_c^-)^{n-1} (c_1 \eta_{j,1,c}^- + c_2 \eta_{j,2,c}^-) \\ &\quad + (\rho_s^+)^{n-1} \left( c_1 \frac{\gamma_s^+}{\delta_s^+} + c_2 \right) \eta_{j,2,s}^+ + (\rho_s^-)^{n-1} (c_1 \eta_{j,1,s}^- + c_2 \eta_{j,2,s}^-). \end{aligned}$$

Taking its  $L^2(0, 1)$ -norm, we have the estimates

$$\begin{aligned} &\|y_{n,j}\|_{L^2(0,1)}^2 \\ &= \left\| (\rho_c^+)^{n-1} \left( \frac{c_1\gamma_c^+ + c_2\delta_c^+}{\delta_c^+} \right) \eta_{j,2,c}^+ + (\rho_s^+)^{n-1} \left( \frac{c_1\gamma_s^+ + c_2\delta_s^+}{\delta_s^+} \right) \eta_{j,2,s}^+ \right\|_{L^2(0,1)}^2 \\ &\quad + o(|\rho_c^+|^{2(n-1)}) + o(|\rho_s^+|^{2(n-1)}) \\ &\geq \left| |\rho_c^+|^{n-1} \left| \frac{c_1\gamma_c^+ + c_2\delta_c^+}{\delta_c^+} \right| \|\eta_{j,2,c}^+\|_{L^2(0,1)}^2 - |\rho_s^+|^{n-1} \left| \frac{c_1\gamma_s^+ + c_2\delta_s^+}{\delta_s^+} \right| \|\eta_{j,2,s}^+\|_{L^2(0,1)}^2 \right| \\ &\quad + o(|\rho_c^+|^{2(n-1)}) + o(|\rho_s^+|^{2(n-1)}). \end{aligned}$$

as  $n \rightarrow \infty$ . Since the coefficients  $c_1\gamma_c^+ + c_2\delta_c^+$  and  $c_1\gamma_s^+ + c_2\delta_s^+$  do not equal to 0 simultaneously for any  $(c_1, c_2) \in \mathbb{C}^2 \setminus \{(0, 0)\}$  due to Lemma 4.9, we see that  $\|y_{n,j}\|_{L^2(0,1)}^2$  grows exponentially as  $n \rightarrow \infty$  in any cases where

$$(i) |\rho_c^+| > |\rho_s^+| (> 1) \quad (ii) |\rho_c^+| = |\rho_s^+| (> 1) \quad (iii) (1 <) |\rho_c^+| < |\rho_s^+|.$$

So,  $y$  is neither an eigenfunction nor an generalized eigenfunction. As a result, we have  $\lambda \in \rho(H^b(\mu))$ .  $\square$

Next, we discuss the proof of Theorem 1.2. We prepare two classes:

$$\sigma_A = \{\lambda \in D_4^- \mid m_{12}(\lambda) \neq 0\} \quad \text{and} \quad \sigma_B = \{\lambda \in D_4^- \mid m_{12}(\lambda) = 0\}.$$

In both cases, it is a key to examine whether or not the coefficients  $\delta_c^-, \delta_s^-, \gamma_c^-, \gamma_s^-$  vanish in the expansion (4.2) and (4.3) because of Lemma 4.5 (ii). First, we study the first class  $\sigma_A$ .

LEMMA 4.10. *Let  $\lambda \in \sigma_A$  and  $\mu \in S^1 \setminus \{0\}$ . Then, we have  $\delta_c^- \neq 0$  and  $\delta_s^- \neq 0$ . Furthermore, we have the followings:*

- ① If  $3\Delta + \Delta_- = 0$  and  $\frac{2}{3}\pi < |\mu| \leq \pi$ , then  $\gamma_c^- = 0$  and  $\gamma_s^- = 0$ .
- ② If  $3\Delta + \Delta_- = 0$  and  $0 < |\mu| < \frac{2}{3}\pi$ , then  $\gamma_c^- = 0$  and  $\gamma_s^- \neq 0$ .
- ③ If  $3\Delta + \Delta_- \neq 0$ , then  $\gamma_c^- \neq 0$  and  $\gamma_s^- \neq 0$ .

*Proof.* In a similar way to (4.7)–(4.10) in Lemma 4.6, we have

$$\tilde{\gamma}_s^- := \det(\mathbf{w}_c^+ \mathbf{w}_c^- \mathbf{w}_s^+ \mathbf{e}_1) = \frac{e^{i\mu} \varphi_1 |\mathbf{x}_c^+ \mathbf{x}_c^-|}{2ie^{-\frac{i\mu}{4}} \sin \frac{\mu}{4}} \left( d_s - \sqrt{D_s} + 8 \sin^2 \frac{\mu}{4} \right), \quad (4.12)$$

$$\tilde{\gamma}_c^- := \det(\mathbf{w}_c^+ \mathbf{e}_1 \mathbf{w}_s^+ \mathbf{w}_s^-) = \frac{e^{i\mu} \varphi_1 |\mathbf{x}_s^+ \mathbf{x}_s^-|}{2e^{-\frac{i\mu}{4}} \cos \frac{\mu}{4}} \left( d_c - \sqrt{D_c} + 8 \cos^2 \frac{\mu}{4} \right), \quad (4.13)$$

$$\tilde{\delta}_s^- := \det(\mathbf{w}_c^+ \mathbf{w}_c^- \mathbf{w}_s^+ \mathbf{e}_2) = -2e^{\frac{i\mu}{2}} |\mathbf{x}_c^+ \mathbf{x}_c^-| (1 + e^{-\frac{i\mu}{2}}) m_{12} \neq 0, \quad (4.14)$$

$$\tilde{\delta}_c^- := \det(\mathbf{w}_c^+ \mathbf{e}_2 \mathbf{w}_s^+ \mathbf{w}_s^-) = 2e^{\frac{i\mu}{2}} |\mathbf{x}_s^+ \mathbf{x}_s^-| (1 - e^{-\frac{i\mu}{2}}) m_{12} \neq 0. \quad (4.15)$$

Due to  $\lambda \in \sigma_A$ , we are dealing with the case of  $m_{12} \neq 0$ . Thus, we have  $\delta_c^- \neq 0$  and  $\delta_s^- \neq 0$  by (4.14) and (4.15) utilizing the Cramer's rule.

We claim the following assertions:

- (1)  $d_s - \sqrt{D_s} + 8 \sin^2 \frac{\mu}{4} = 0$  is equivalent to  $9\Delta^2 - \Delta_-^2 = 0$  and  $\frac{2}{3}\pi < |\mu| \leq \pi$ .
- (2)  $d_c - \sqrt{D_c} + 8 \cos^2 \frac{\mu}{4} = 0$  is equivalent to  $9\Delta^2 - \Delta_-^2 = 0$ .

First, we prove (1). Assume that  $d_s - \sqrt{D_s} + 8 \sin^2 \frac{\mu}{4} = 0$ . Squaring  $\sqrt{D_s} = d_s + 8 \sin^2 \frac{\mu}{4}$ , we have  $d_s = -1 - 4 \sin^2 \frac{\mu}{4}$ , namely,  $9\Delta^2 - \Delta_-^2 = 0$ . This is why  $D_s = (4 \sin^2 \frac{\mu}{4} - 1)^2$ . Substituting this into  $\sqrt{D_s} = d_s + 8 \sin^2 \frac{\mu}{4}$ , we have  $-1 + 4 \sin^2 \frac{\mu}{4} = |4 \sin^2 \frac{\mu}{4} - 1|$ , which yields  $-1 + 4 \sin^2 \frac{\mu}{4} \geq 0$ . Hence,  $\frac{2}{3}\pi \leq |\mu| \leq \pi$ . Due to  $D_s > 0$ , we have to exclude the case of  $|\mu| = \frac{2}{3}\pi$ . Therefore, we have  $\frac{2}{3}\pi < |\mu| \leq \pi$ . Conversely, we assume that  $9\Delta^2 - \Delta_-^2 = 0$  and  $\frac{2}{3}\pi < |\mu| \leq \pi$ . It follows by  $9\Delta^2 - \Delta_-^2 = 0$  that  $d_s = -1 - 4 \sin^2 \frac{\mu}{4}$  and  $D_s = (4 \sin^2 \frac{\mu}{4} - 1)^2$ . It turns out by  $\frac{2}{3}\pi < |\mu| \leq \pi$  that  $4 \sin^2 \frac{\mu}{4} - 1 > 0$ . So, we derive  $d_s - \sqrt{D_s} + 8 \sin^2 \frac{\mu}{4} = -1 - 4 \sin^2 \frac{\mu}{4} - (4 \sin^2 \frac{\mu}{4} - 1) + 8 \sin^2 \frac{\mu}{4} = 0$ . Therefore, we obtain (1).

Next, we prove (2). Assume that  $d_c - \sqrt{D_c} + 8 \cos^2 \frac{\mu}{4} = 0$ . In the case, we have  $d_c = -1 - 4 \cos^2 \frac{\mu}{4}$ . This implies  $9\Delta^2 - \Delta_-^2 = 0$ . Conversely, we assume that  $9\Delta^2 - \Delta_-^2 = 0$ . Then, we have  $d_c = -1 - 4 \cos^2 \frac{\mu}{4}$  and  $D_c = (4 \cos^2 \frac{\mu}{4} - 1)^2$ . For any  $\mu \in S^1 \setminus \{0\} = [-\pi, 0) \cup (0, \pi)$ , we have  $4 \cos^2 \frac{\mu}{4} > 1$ . Thus, we have  $\sqrt{D_c} = 4 \cos^2 \frac{\mu}{4} - 1$ . So, we obtain  $d_c - \sqrt{D_c} + 8 \cos^2 \frac{\mu}{4} = 0$ .

Since  $m_{12} = 0$  is equivalent to  $3\Delta - \Delta_- = 0$ , we see that  $9\Delta^2 - \Delta_-^2 = 0$  is equivalent to  $3\Delta - \Delta_- = 0$  for  $\lambda \in \sigma_A$ . Therefore, we have ①, ② and ③.  $\square$

*Proof of Theorem 1.2 (A) and (B).* Assume that  $\mu \in S^1 \setminus \{0, \pm \frac{2}{3}\pi, \pm \pi\}$  and  $\lambda \in \sigma_A$ . First, we prove (B). Assume that  $3\Delta + \Delta_- \neq 0$ . Lemma 4.9 yields

$$-\tilde{\delta}_c^- \tilde{\gamma}_s^- + \tilde{\delta}_s^- \tilde{\gamma}_c^- = 2e^{\frac{3i\mu}{2}} m_{12} \varphi_1 |\mathbf{x}_s^+ \mathbf{x}_s^-| |\mathbf{x}_c^+ \mathbf{x}_c^-| (d_s - \sqrt{D_s} + d_c - \sqrt{D_c} + 8).$$

Then, we have the followings:

- (a) If  $\lambda$  satisfies  $d_s - \sqrt{D_s} + d_c - \sqrt{D_c} + 8 \neq 0$ , we have  $(c_1 \gamma_c^- + c_2 \delta_c^-, c_1 \gamma_s^- + c_2 \delta_s^-) \neq (0, 0)$  for any  $(c_1, c_2) \in \mathbb{C}^2 \setminus \{(0, 0)\}$ .

(b) If  $\lambda$  satisfies  $d_s - \sqrt{D_s} + d_c - \sqrt{D_c} + 8 = 0$ , we have  $\delta_c^- \gamma_s^- - \delta_s^- \gamma_c^- = 0$ .

The statement (a) can be proven in a similar way to Lemma 4.9.

If  $\lambda$  satisfies  $d_s - \sqrt{D_s} + d_c - \sqrt{D_c} + 8 \neq 0$ , we obtain the estimate

$$\begin{aligned} \|y_{n,j}\|_{L^2(0,1)}^2 &\geq \left| |\rho_c^-|^{n-1} \left| \frac{c_1 \gamma_c^- + c_2 \delta_c^-}{\delta_c^-} \right| \|\eta_{j,2,c}^-\|_{L^2(0,1)}^2 \right. \\ &\quad \left. - |\rho_s^-|^{n-1} \left| \frac{c_1 \gamma_s^- + c_2 \delta_s^-}{\delta_s^-} \right| \|\eta_{j,2,s}^-\|_{L^2(0,1)}^2 \right|^2 \\ &\quad + o(|\rho_c^-|^{2(n-1)}) + o(|\rho_s^-|^{2(n-1)}) \end{aligned}$$

in a similar way to the proof of Theorem 1.1 (4). So, we have (B-1).

Assume that  $\lambda$  satisfies  $d_s - \sqrt{D_s} + d_c - \sqrt{D_c} + 8 = 0$ . Recall that  $\gamma_c^- \neq 0$  and  $\gamma_s^- \neq 0$  from Lemma 4.10. Using  $\delta_c^- \mathbf{e}_{1,c} - \gamma_c^- \mathbf{e}_{2,c} = \mathbf{o}$ , we have  $\delta_c^- \alpha_{j,1,c}^- - \gamma_c^- \alpha_{j,2,c}^- = 0$  and  $\delta_c^- \beta_{j,1,c}^- - \gamma_c^- \beta_{j,2,c}^- = 0$  for all  $j = 1, 2, 3, 4, 5, 6$ . So, we have  $\delta_c^- \eta_{j,1,c}^- - \gamma_c^- \eta_{j,2,c}^- = 0$  for all  $j$ . In a similar way, we also have  $\delta_s^- \eta_{j,1,s}^- - \gamma_s^- \eta_{j,2,s}^- = 0$  for all  $j$ . Substituting  $\delta_c^- = \frac{\gamma_c^-}{\gamma_s^-} \delta_s^-$  into  $\delta_c^- \eta_{j,1,c}^- - \gamma_c^- \eta_{j,2,c}^- = 0$ , we derive  $\delta_s^- \eta_{j,1,c}^- - \gamma_s^- \eta_{j,2,c}^- = 0$  for all  $j$ . Therefore, we have  $(c_1 \eta_{j,1,c}^- + c_2 \eta_{j,2,c}^-, c_1 \eta_{j,1,s}^- + c_2 \eta_{j,2,s}^-) = (0, 0)$  for  $(c_1, c_2) = (\delta_s^-, -\gamma_s^-) \neq (0, 0)$ . For such a pair  $(c_1, c_2)$ , we have  $\|y\|_{L^2(\Gamma_0^b)} < +\infty$ . So, we have  $\lambda \in \sigma_p(H^b(\mu))$ . Hence, (B-2) has been established.

Next, we prove (A). We discuss the case of  $3\Delta + \Delta_- = 0$  and  $0 < |\mu| < \frac{2}{3}\pi$ . Then, we recall  $\gamma_c^- = 0$  from Lemma 4.10. This implies  $\mathbf{e}_{1,c}^- = \mathbf{o}$ . Thus, it turns out by (3.7)–(3.9) that  $\alpha_{j,1,c}^- = \beta_{j,1,c}^- = 0$  for  $j = 1, 2, 3, 4, 5, 6$ . This yields  $\eta_{j,1,c}^- \equiv 0$  for all  $j = 1, 2, 3, 4, 5, 6$  (see Lemma 3.4 (1)). Therefore, we have the estimates

$$\begin{aligned} \|y_{n,j}\|_{L^2(0,1)}^2 &\geq \left| |\rho_c^-|^{n-1} |c_2| \|\eta_{j,2,c}^-\|_{L^2(0,1)}^2 - |\rho_s^-|^{n-1} \left| \frac{c_1 \gamma_s^- + c_2 \delta_s^-}{\delta_s^-} \right| \|\eta_{j,2,s}^-\|_{L^2(0,1)}^2 \right|^2 \\ &\quad + o(|\rho_c^-|^{2(n-1)}) + o(|\rho_s^-|^{2(n-1)}) \end{aligned}$$

Due to  $\gamma_s^- \neq 0$ , we see that  $(c_2, c_1 \gamma_s^- + c_2 \delta_s^-) \neq (0, 0)$  for any  $(c_1, c_2) \in \mathbb{C}^2 \setminus \{(0, 0)\}$ . So, we have  $\lambda \in \rho(H^b(\mu))$ .

At last, we deal with the case of  $3\Delta + \Delta_- = 0$  and  $\frac{2}{3}\pi < |\mu| < \pi$  (Note that  $\frac{2}{3}\pi < |\mu| \leq \pi$  can be permitted.). In the case, we derived  $\gamma_c^- = 0$  and  $\gamma_s^- = 0$ . Then, we have  $\eta_{j,1,c}^- \equiv 0$  and  $\eta_{j,1,s}^- \equiv 0$ . Looking at Lemma 3.4 (2), we have

$$\|p_{n,j}\|_{L^2(0,1)}^2 \leq 2(|\rho_c^+|^{2(n-1)} \|\eta_{j,1,c}^+\|_{L^2(0,1)}^2 + |\rho_s^+|^{2(n-1)} \|\eta_{j,1,s}^+\|_{L^2(0,1)}^2).$$

This means that  $\lambda$  is an eigenvalue of  $H^b(\mu)$  and  $p$  is an eigenfunction corresponding to  $\lambda$ . (On the other hand,  $q$  is neither an eigenfunction nor a generalized eigenfunction.) This is why we derive  $\lambda \in \sigma_p(H^b(\mu))$ .  $\square$

Finally, we discuss the proof of Theorem 1.2 (C) and (D). Since all discussions so far was corresponding to the case of  $m_{12} \neq 0$ , we were using Lemma 2.4 (1) as

eigenspaces for the transfer matrix  $M(\lambda)$ . From now on, we utilize the expression in Lemma 2.4 (2) under the setting  $\lambda \in \sigma_B$ . Recall that  $\lambda \in \sigma_B$  is equivalent to  $\varphi'_1 + 2\Delta = 0$ , namely,  $\varphi'_1 = -\frac{\theta_1}{2}$ .

LEMMA 4.11. Assume that  $\lambda \in \sigma_B$  and  $\mu \in S^1 \setminus \{0\}$ . Then,  $\delta_c^- \neq 0$ .

(1) The potential  $q$  is even if and only if  $\gamma_c^- = 0$ .

(2-a) Assume that  $0 < |\mu| < \frac{2}{3}\pi$ . Then,  $\gamma_s^- \neq 0$  and  $\delta_s^- = 0$ .

(2-b) Assume that  $\frac{2}{3}\pi < |\mu| \leq \pi$ . Then,  $\delta_s^- \neq 0$ . Moreover,  $q$  is even if and only if  $\gamma_s^- = 0$ .

*Proof.* We calculate the 2nd row of  $\mathbf{x}_c^+$  in Lemma 2.4 (2). Using  $m_{11}$  in Lemma 2.1, we have

$$\begin{aligned} 2\Delta m_{11}(e^{-\frac{i\mu}{2}} - 1) + \theta_1(e^{\frac{i\mu}{2}} + 1) &= e^{\frac{i\mu}{4}} \left( \frac{-\varphi'_1}{2\cos\frac{\mu}{4}} + 2\theta_1 \cos\frac{\mu}{4} \right) \\ &= 2\theta_1 e^{\frac{i\mu}{4}} \left( \cos\frac{\mu}{4} + \frac{1}{8\cos\frac{\mu}{4}} \right) \end{aligned}$$

because of  $\varphi'_1 = -\frac{\theta_1}{2}$ . Since  $\rho_c^+ + 1 + e^{\frac{i\mu}{2}} = e^{\frac{i\mu}{4}}(2\cos\frac{\mu}{4} - \frac{1}{2\cos\frac{\mu}{4}}) \neq 0$ , we have

$$|\mathbf{x}_c^+ \mathbf{e}_1^+| = 3\theta_1 \varphi_1 e^{\frac{i\mu}{4}} \cos\frac{\mu}{4}.$$

Hence, we see that  $|\mathbf{x}_c^+ \mathbf{e}_1^+| = 0$  is equivalent to  $\theta_1 = 0$ , which is moreover equivalent to  $\Delta_- = 0$  because of  $\varphi'_1 = -\frac{\theta_1}{2}$ . Recall that  $\Delta_-$  plays the role to determine whether or not  $q$  is even. This is why (4.4) and (4.5) mean that  $\gamma_c^- = 0$  is equivalent to  $q$  is even.

Next, we prove that  $\delta_c^- \neq 0$ . Note that

$$\tilde{\delta}_c^- := \det(\mathbf{w}_c^+ \mathbf{e}_2 \mathbf{w}_s^+ \mathbf{w}_s^-) = 2e^{\frac{i\mu}{2}} |\mathbf{x}_c^+ \mathbf{x}_s^-| \varphi_1(\rho_c^+ + 1 + e^{\frac{i\mu}{2}}). \quad (4.16)$$

This combined with  $\rho_c^+ + 1 + e^{\frac{i\mu}{2}} \neq 0$  yields  $\delta_c^- \neq 0$ .

Finally, we show (2-a) and (2-b) using the expressions in Lemma 2.4 (2). If  $0 < |\mu| < \frac{2}{3}\pi$ , then we have the following statements, which mean (2-a):

$$\det(\mathbf{w}_c^+ \mathbf{w}_c^- \mathbf{w}_s^+ \mathbf{e}_1) = 2e^{i\mu} |\mathbf{x}_c^+ \mathbf{x}_c^-| |\mathbf{e}_2^- \mathbf{e}_1^+| \neq 0,$$

$$\det(\mathbf{w}_c^+ \mathbf{w}_c^- \mathbf{w}_s^+ \mathbf{e}_2) = 2e^{i\mu} |\mathbf{x}_c^+ \mathbf{x}_c^-| |\mathbf{e}_2^- \mathbf{e}_2^-| = 0.$$

If  $\frac{2}{3}\pi < |\mu| \leq \pi$ , then we have

$$\tilde{\gamma}_s^- := \det(\mathbf{w}_c^+ \mathbf{w}_c^- \mathbf{w}_s^+ \mathbf{e}_1) = 2e^{i\mu} |\mathbf{x}_c^+ \mathbf{x}_c^-| |\mathbf{x}_s^+ \mathbf{e}_1^+|, \quad (4.17)$$

$$\tilde{\delta}_s^- := \det(\mathbf{w}_c^+ \mathbf{w}_c^- \mathbf{w}_s^+ \mathbf{e}_2) = -2e^{i\mu} |\mathbf{x}_c^+ \mathbf{x}_c^-| |\mathbf{x}_s^+ \mathbf{e}_2^-|. \quad (4.18)$$

Since we have  $|\mathbf{x}_s^+ \mathbf{e}_1^+| = -3\theta_1 \varphi_1 i e^{\frac{i\mu}{4}} \sin \frac{\mu}{4}$ , we see that  $\gamma_s^- = 0$  if and only if  $q$  is even. It follows by  $|\mathbf{x}_s^+ \mathbf{e}_2^-| = \varphi_1(\rho_s^+ + 1 - e^{\frac{i\mu}{2}}) \neq 0$  that  $\delta_s^- \neq 0$ .  $\square$

*Proof of Theorem 1.2 (C) and (D).* Assume that  $\mu \in S^1 \setminus \{0, \pm \frac{2}{3}\pi, \pm \pi\}$  and  $\lambda \in \sigma_B$ . Recall  $|\rho_s^+| < 1$ ,  $|\rho_c^+| < 1$ ,  $|\rho_s^-| > 1$ ,  $|\rho_c^-| > 1$  from Lemma 4.5 (ii). We prepare the following classifications for the proof:

(C-1)  $q$  is even and  $0 < |\mu| < \frac{2}{3}\pi$ . (C-2)  $q$  is even and  $\frac{2}{3}\pi < |\mu| < \pi$ .

(D-1)  $q$  is not even and  $0 < |\mu| < \frac{2}{3}\pi$ . (D-2)  $q$  is not even and  $\frac{2}{3}\pi < |\mu| < \pi$ .

Consider the case (C-1). Then, it follows by Lemma 4.11 that  $\gamma_c^- = 0$ ,  $\gamma_s \neq 0$ ,  $\delta_c^- \neq 0$  and  $\delta_s^- = 0$ . Therefore, we have  $\mathbf{e}_{1,c}^- = \mathbf{e}_{2,s}^- = \mathbf{o}$  in the eigenfunction expansion (4.2) and (4.3). This implies by the notations (3.7)–(3.9) that  $\alpha_{j,1,c}^- = \beta_{j,1,c}^- = \alpha_{j,2,s}^- = \beta_{j,2,s}^- = 0$  for all  $j = 1, 2, 3, 4, 5, 6$ . Recall the definition of  $\eta_{j,\ell,\bullet}^\pm$  from Lemma 3.4 (1). As a result, we have  $\eta_{j,1,c}^-(x, \lambda) \equiv 0$  and  $\eta_{j,2,s}^-(x, \lambda) \equiv 0$  for  $j = 1, 2, 3, 4, 5, 6$ . Therefore, we have

$$\|y_{n,j}\|_{L^1(0,1)}^2 = \|c_1(\rho_s^-)^{n-1}\eta_{j,1,s}^- + c_2(\rho_c^-)^{n-1}\eta_{j,2,c}^-\|_{L^2(0,1)}^2 + o(|\rho_c^-|^{2(n-1)}) + o(|\rho_s^-|^{2(n-1)})$$

as  $n \rightarrow \infty$  by Lemma 3.4 (1). For any  $(c_1, c_2) \in \mathbb{C}^2 \setminus \{(0, 0)\}$ ,  $\|y_{n,j}\|_{L^2(0,1)}^2$  grows exponentially in all cases (i)  $|\rho_s^-| > |\rho_c^-| (> 1)$ , (ii)  $|\rho_s^-| = |\rho_c^-| (> 1)$  and (iii)  $(1 <) |\rho_s^-| < |\rho_c^-|$ . Since any non-trivial solution can be neither an eigenfunction nor a generalized eigenfunction, we have  $\lambda \in \rho(H^b(\mu))$ .

Consider the case (C-2). By Lemma 4.11, we have  $\gamma_c^- = 0$ ,  $\gamma_s^- = 0$ ,  $\delta_c^- \neq 0$  and  $\delta_s^- \neq 0$ . Then, we have  $\eta_{j,1,c}^-(x, \lambda) \equiv 0$  and  $\eta_{j,1,s}^-(x, \lambda) \equiv 0$  for all  $j = 1, 2, 3, 4, 5, 6$ . Substituting these into Lemma 3.4 (2), we have  $p_{n,j} = (\rho_c^+)^{n-1}\eta_{j,1,c}^+ + (\rho_s^+)^{n-1}\eta_{j,1,s}^+$ . This yields  $\|p\|_{L^2(\Gamma^b)} < \infty$  which means that  $\lambda \in \sigma_p(H^b(\mu))$  and  $p$  is its corresponding eigenfunction.

We deal with the case (D-1). In this case, we have  $\gamma_c^- \neq 0$ ,  $\gamma_s^- \neq 0$ ,  $\delta_c^- \neq 0$  and  $\delta_s^- = 0$ . Then, we have  $\eta_{j,2,s}^-(x, \lambda) \equiv 0$ . On the other hand, it follows by  $\gamma_c^- \mathbf{w}_c^- = \mathbf{e}_{1,c}^- \neq 0$  and  $\delta_c^- \mathbf{w}_c^- = \mathbf{e}_{2,c}^- \neq 0$  that  $\mathbf{e}_{1,c}^- = \frac{\gamma_c^-}{\delta_c^-} \mathbf{e}_{2,c}^-$ . From the point of view of the notations in (3.7)–(3.9), we have  $\alpha_{j,1,c}^- = \frac{\gamma_c^-}{\delta_c^-} \alpha_{j,2,c}^-$  and  $\beta_{j,1,c}^- = \frac{\gamma_c^-}{\delta_c^-} \beta_{j,2,c}^-$ , which yield  $\eta_{j,1,c}^- = \frac{\gamma_c^-}{\delta_c^-} \eta_{j,2,c}^-$  for  $j = 1, 2, 3, 4, 5, 6$ . Thus, we have

$$\begin{aligned} \|y_{n,j}\|_{L^2(0,1)}^2 &= \|(\rho_c^-)^{n-1} \left( \frac{c_1 \gamma_c^- + c_2 \delta_c^-}{\delta_c^-} \right) \eta_{j,2,c}^- + (\rho_s^-)^{n-1} c_1 \eta_{j,1,s}^-\|_{L^2(0,1)}^2 \\ &\quad + o(|\rho_c^-|^{2(n-1)}) + o(|\rho_s^-|^{2(n-1)}) \end{aligned}$$

as  $n \rightarrow \infty$ . For any  $(c_1, c_2) \in \mathbb{C}^2 \setminus \{(0, 0)\}$ , we see that  $(c_1 \gamma_c^- + c_2 \delta_c^-, c_1) \neq (0, 0)$ . Thus,  $\|y_{n,j}\|_{L^2(0,1)}^2$  grows exponentially as  $n \rightarrow \infty$  in all cases (i)  $|\rho_s^-| > |\rho_c^-|$ , (ii)  $|\rho_s^-| = |\rho_c^-|$  and (iii)  $|\rho_s^-| < |\rho_c^-|$ . Hence, we have  $\lambda \in \rho(H^b(\mu))$ .



Consider the case (D-2). At last, we finish so many classifications. In the case, we have  $\gamma_c^- \neq 0$ ,  $\gamma_s^- \neq 0$ ,  $\delta_c^- \neq 0$  and  $\delta_s^- \neq 0$ . Then, we have  $\eta_{j,1,c}^- = \frac{\gamma_c^-}{\delta_c^-} \eta_{j,2,c}^-$  and  $\eta_{j,1,s}^- = \frac{\gamma_s^-}{\delta_s^-} \eta_{j,2,s}^-$ . Hence, it follows by Lemma 3.4 (1) that

$$y_{n,j}(x, \lambda) = (\rho_c^+)^{n-1} (c_1 \eta_{j,1,c}^+ + c_2 \eta_{j,2,c}^+) + (\rho_s^+)^{n-1} (c_1 \eta_{j,1,s}^+ + c_2 \eta_{j,2,s}^+) \\ + (\rho_c^-)^{n-1} \left( \frac{c_1 \gamma_c^- + c_2 \delta_c^-}{\delta_c^-} \right) \eta_{j,2,c}^- + (\rho_s^-)^{n-1} \left( \frac{c_1 \gamma_s^- + c_2 \delta_s^-}{\delta_s^-} \right) \eta_{j,2,s}^-.$$

Our last task is to show that  $(c_1 \gamma_s^- + c_2 \delta_c^-, c_1 \gamma_s^- + c_2 \delta_s^-) \neq (0, 0)$  for any  $(c_1, c_2) \in \mathbb{C}^2 \setminus \{(0, 0)\}$ . Seeking a contradiction, we assume that there exists some  $(c_1, c_2) \in \mathbb{C}^2 \setminus \{(0, 0)\}$  satisfying  $c_1 \gamma_c^- + c_2 \delta_c^- = c_1 \gamma_s^- + c_2 \delta_s^- = 0$ . This is equivalent to  $\tilde{\gamma}_c^- \delta_s^- - \tilde{\gamma}_s^- \delta_c^- = 0$ . Substituting (4.5), (4.16), (4.17) and (4.18) into this, we have  $\cos \mu = 0$ . This does not hold true for  $\frac{2}{3}\pi < |\mu| < \pi$ . Therefore, we have  $(c_1 \gamma_s^- + c_2 \delta_c^-, c_1 \gamma_s^- + c_2 \delta_s^-) \neq (0, 0)$  for any  $(c_1, c_2) \in \mathbb{C}^2 \setminus \{(0, 0)\}$ . As a result, we see that the  $L^2(0, 1)$ -norm of any non-trivial solution  $y$  in Lemma 3.4 grows exponentially. Namely,  $\lambda \in \rho(H^b(\mu))$ .  $\square$

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## REFERENCES

- [1] G. BERKOLAIKO AND P. KUCHMENT, *Introduction to quantum graphs*, AMS, Providence, RI (2012).
- [2] M. S. P. EASTHAM, *The spectral theory of periodic differential equations*, Scottish Academic Press Ltd., London, 1973.
- [3] G. M. GRAF AND M. PORTA, *Bulk-Edge Correspondence for Two-Dimensional Topological Insulators*, Commun. Math. Phys., **324**, 851–895 (2013).
- [4] C. L. KANE AND E. J. MALE,  $\mathbb{Z}_2$  Topological order and the quantum spin Hall effect, Phys. Rev. Lett., **95**, 146802 (2005).
- [5] E. KOROTYAEV AND I. LOBANOV, *Schrödinger Operators on Zigzag Nanotubes*, Ann. Henri Poincaré **8**, 1151–1176 (2007).
- [6] E. KOROTYAEV AND N. SABUROVA, *Scattering on metric graphs*, Rev. Math. Phys. **32**, no. 8, 2050025 (51 pp) (2020).
- [7] W. MAGNUS AND S. WINKLER, *Hill's Equation*, Wiley (1966).
- [8] H. NIHKUNI, *Edge states of Schrödinger equations on graphene with zigzag boundaries*, Results Math. **76** (2021), no. 2, Paper No. 55, 26 pp.
- [9] J. POSCHEL AND E. TRUBOWITZ, *Inverse Spectral Theory*, Academic Press, Orlando (1987).
- [10] M. REED AND B. SIMON, *Methods of modern mathematical physics, IV. Analysis of operators*, Academic Press, New York (1978).

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