Spectral discriminants for a variant graphene with bumpy boundaries

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1 Introduction

We discussed the spectral structure for a quantum graph corresponding to a variant graphene with bumpy boundaries in the RIMS Workshop "Spectral and Scattering Theory and Related Topics" on 1st December, 2021. The topic is based on the paper [4]. In this note, we report the statements which we shared in the workshop. We note that the proof of theorems in this note is described in [3, 4]. The spectral analysis for materials with boundaries draws our attentions from the point of view of topological insulators. Topological Insulators behave as insulators in their interior (**Bulk**), but their surface (**Edge**) contains conducting states. This properties can be found in the spectral analysis of a Bulk Hamiltonian and Edge Hamiltonian as an energy located in the spectral gaps of a periodic media, but in the absolutely continuous spectrum of the periodic media with boundaries. Thus, it is important to compare the spectral structure of Schrödinger operators in the whole space without boundaries and the half space with boundaries.

For example, Graf and Porta [2] considered

- **the k-parametrized bulk Hamiltonian**

$$(H_{GP}\psi)_n = A(k)\psi_{n-1} + A(k)^*\psi_{n+1} + V_n(k)\psi_n, \quad n \in \mathbb{Z}$$

  for $\psi = (\psi_n)_{n\in\mathbb{Z}} \in \ell^2(\mathbb{Z};\mathbb{C}^N)$, $k \in S^1 := [-\pi,\pi)$ and

- the k**-parametrized edge Hamiltonian**

$$(H^\sharp_{GP}\psi)_n = A(k)\psi_{n-1} + A(k)^*\psi_{n+1} + V^\sharp_n(k)\psi_n, \quad n \in \mathbb{N}$$

  for $\psi = (\psi_n)_{n\in\mathbb{N}} \in \ell^2(\mathbb{N};\mathbb{C}^N)$ with $\psi_0 = 0$.

Here, $A(k), V_n(k), V^\sharp_n(k)$ are suitable $N\times N$ matrices. They constructed 2 indices (Bulk Index and Edge Index) and their correspondence (Bulk-Edge Correspondence). Putting

$$N = 2, \quad \psi_n = \begin{pmatrix} \psi_n^A \\ \psi_n^B \end{pmatrix}, \quad n = n_1, \quad A(k) = -\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \quad \text{and} \quad V(k) = -\begin{pmatrix} 0 & 1+e^{-ik} \\ 1+e^{ik} & 0 \end{pmatrix},$$

their model corresponds to fiber operators for Bulk and Edge Hamiltonians on graphene:

$$(H_{\mathrm{G}}(k)\psi)_n := A(k)\psi_{n-1} + A(k)^*\psi_{n+1} + V_n(k)\psi_n = -\begin{pmatrix} \psi^B_{n_1-1} + (1+e^{-ik})\psi^B_{n_1} \\ \psi^A_{n_1+1} + (1+e^{ik})\psi^A_{n_1} \end{pmatrix}.$$

The operator $H_{\mathrm{G}}(k)$ is a fiber operator of the standard Laplacian on Graphene:

$$\begin{cases} (H_G\psi)^{\mathrm{A}}_{n_1,n_2} := -(\psi^{\mathrm{B}}_{n_1,n_2} + \psi^{\mathrm{B}}_{n_1,n_2-1} + \psi^{\mathrm{B}}_{n_1-1,n_2}), \\ (H_G\psi)^{\mathrm{B}}_{n_1,n_2} := -(\psi^{\mathrm{A}}_{n_1,n_2+1} + \psi^{\mathrm{A}}_{n_1+1,n_2} + \psi^{\mathrm{A}}_{n_1,n_2}), \end{cases}$$

In this study, we consider Schrödinger operators on variant graphenes with bumpy boundaries (Fig. 1) from the point of view of quantum graphs [1] and discuss their spectra. This note is organized as follows:

Section 1. From the point of view of the quantum graph, we define our Schrödinger operator and introduce its fiber operators.

Section 2. We state main results.
1) Introduce spectral discriminants $D_s(\mu,\lambda)$ and $D_c(\mu,\lambda)$.
2) State main theorems.
3) Draw a picture of Dispersion Relations numerically.
4) Compare the graphene with zigzag boundaries with the variant graphene with bumpy boundaries.

Section 3. We state an outline of the proofs. Especially, we note that Cramer's Rule works to determine the spectrum.

We state the definition of our quantum graph corresponding to the variant graphene with bumpy boundaries seen in Fig. 1. Let $\Gamma^\flat = (E^\flat, V^\flat)$ be the metric graph appearing in Fig. 1. Here, $E^\flat$ and $V^\flat$ are the set of edges and vertexes of $\Gamma^\flat$. Each vertex in $V^\flat$ is uniquely identified by the labels $A(n,k), B(n,k), C(n,k)$ and $D(n,k)$ as seen in Fig. 1. Furthermore, we assume the followings:

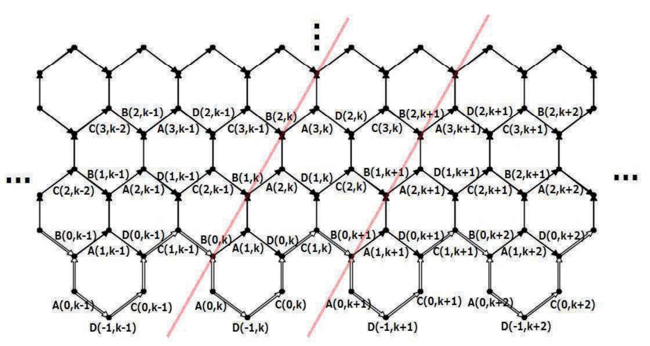

Figure 1: variant graphenes with bumpy boundaries

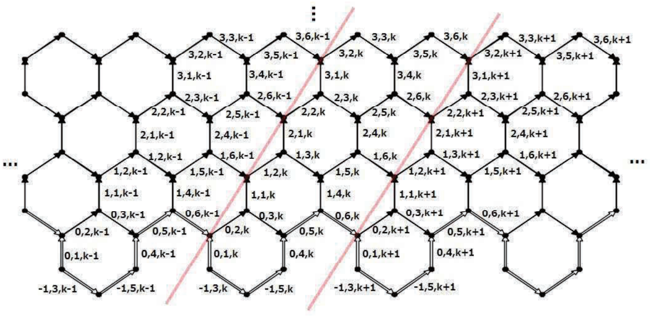

Figure 2: The definition of index (n, j, k) of each edge $e \in E^\flat$.

(1) The length of each edge $e \in E^\flat$ is equal to 1.

(2) The potential $q \in L^2(0, 1)$ is real-valued and bounded from the below.

Due to the assumption (1), we identify each edge $e \in E^\flat$ with the interval $(0, 1)$. Under these assumption, we define the variant edge Hamiltonian $H^\flat$ in $L^2(\Gamma^\flat)$ as follows: For any $e \in E^\flat$, the variant edge Hamiltonian $H^\flat$ acts as

$$(H^\flat y)_e(x) = -y_e''(x) + q(x)y_e(x), \quad x \in (0, 1) \simeq e, \tag{1.1}$$

where $y \in \mathrm{Dom}(H^\flat)$ satisfies

(a) the Kirchhoff vertex condition at each $v \in V^\flat \setminus \partial\Gamma^\flat$ and

(b) the Dirichlet boundary condition $y \equiv 0$ on $\partial\Gamma^\flat$.

To explain the Kirchhoff vertex condition, we give an address (n, j, k) as seen in Fig. 2 uniquely to each edge $e \in E^\flat$ and put $y|_{e_{n,j,k}} = y_{n,j,k}$ for a function y on $\Gamma^\flat$. Then, the Kirchhoff vertex condition at $B(n, k)$ is given as

$$y_{n,1,k}(1) = y_{n,2,k}(0) = y_{n,6,k-1}(1), \quad -y'_{n,1,k}(1) + y'_{n,2,k}(0) - y'_{n,6,k-1}(1) = 0.$$

Since $H^\flat$ is periodic with respect to the vector $\mathbf{a}_2 := \overrightarrow{B(0,0)B(0,1)}$, we construct a direct integral decomposition (see [5])

$$H^\flat \simeq \int_{S^1}^{\oplus} H^\flat(\mu)\frac{d\mu}{2\pi},$$

where $\mu \in S^1 := [-\pi, \pi)$ is a quasi-momentum and $H^\flat(\mu)$ is a fiber operator of $H^\flat$ defined as follows. At first, we pick the fundamental domain as in Fig. 3. In Fig. 3, we consider the part of $k = 0$ of $\Gamma^\flat$. In the case of $k = 0$, we dropped the index from each edge. We describe the definition of fiber operators $H^\flat(\mu)$ for $H^\flat$. For $y = (y_{n,j}) \in \mathrm{dom}(H^\flat(\mu))$, the fiber operator $H^\flat(\mu)$ in $L^2(\Gamma_0^\flat)$ acts as

$$(H^\flat(\mu)y)_e(x) = -y_e''(x) + q(x)y_e(x), \quad x \in (0, 1) \simeq e \in E_0^\flat,$$

where $y \in \mathrm{dom}(H^\flat(\mu))$ satisfies

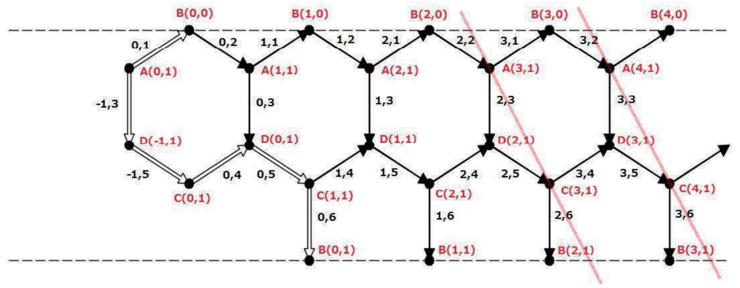

Figure 3: A fundamental domain $\Gamma_0^\flat = (E_0^\flat, V_0^\flat)$

(a) the Kirchhoff vertex condition at $\forall v \in \mathrm{int} V_0^\flat$,

(b) the Dirichlet boundary condition $y \equiv 0$ on $\partial\Gamma^\flat$ and

(c) the quasi-periodic boundary conditions:

$$y_{n,1}(1) = y_{n,2}(0) = e^{-i\mu} y_{n,6}(1), \ -y'_{n,1}(1) + y'_{n,2}(0) - e^{-i\mu} y'_{n,6}(1) = 0.$$

Then, we have the unitarily equivalence (1.1). Let m be the Lebesgue measure on $S^1 := [-\pi, \pi)$. According to [Reed-Simon IV, Section XIII], we have the following spectral correspondence.

(1) $\lambda \in \sigma(H^\flat)$ if and only if $m(\{\mu \in S^1 | \quad \sigma(H^\flat(\mu)) \cap (\lambda - \epsilon, \lambda + \epsilon) \neq \emptyset\}) > 0$ for any $\epsilon > 0$.

(2) $\lambda \in \sigma_p(H^\flat)$ if and only if $m(\{\mu \in S^1 | \quad \lambda \in \sigma_p(H^\flat(\mu))\}) > 0$.

Due to these correspondence, we notice that it suffices to study $\sigma(H^\flat(\mu))$ in order to study $\sigma(H^\flat)$.

2 Main Results

In this section, we introduce the main results from [4]. At first, we prepare notations to describe them. Expand q to the 1-periodic function. Let σ_D be the set of eigenvalues of the spectral problem

$$-y'' + qy = \lambda y \quad \text{on} \quad (0,1) \quad \text{and} \quad y(0) = y(1) = 0.$$

Note that $\sigma_D = \{n^2\pi^2 | \quad n \in \mathbb{N}\}$ if $q \equiv 0$. Moreover, let $\theta(x, \lambda)$ and $\varphi(x, \lambda)$ be the solutions to $-y'' + qy = \lambda y$ in $\mathbb{R}$ satisfying

$$(\theta(0,\lambda), \theta'(0,\lambda)) = (1, 0) \quad \text{and} \quad (\varphi(0,\lambda), \varphi'(0,\lambda)) = (0, 1),$$

respectively. Furthermore, we put

$$\Delta(\lambda) = \frac{\theta(1,\lambda) + \varphi'(1,\lambda)}{2} \quad \text{and} \quad \Delta_-(\lambda) = \frac{\theta(1,\lambda) - \varphi'(1,\lambda)}{2}.$$

If $q \equiv 0$, then

$$\theta(x,\lambda) = \cos x\sqrt{\lambda}, \quad \varphi(x,\lambda) = \frac{\sin x\sqrt{\lambda}}{\sqrt{\lambda}}, \quad \Delta(\lambda) = \cos\sqrt{\lambda} \quad \text{and} \quad \Delta_-(\lambda) = 0.$$

Under these notations, we introduce spectral discriminants for $H^\flat(\mu)$. For each $(\mu,\lambda) \in S^1 \times \mathbb{R}$, we define

$$D_s(\mu,\lambda) = d_s^2(\mu,\lambda) - 16\sin^2\frac{\mu}{4}$$

and

$$D_c(\mu,\lambda) = d_c^2(\mu,\lambda) - 16\cos^2\frac{\mu}{4},$$

where $d_s(\mu,\lambda) = 9\Delta^2(\lambda) - \Delta_-^2(\lambda) - 1 - 4\sin^2\frac{\mu}{4}$ and $d_c(\mu,\lambda) = 9\Delta^2(\lambda) - \Delta_-^2(\lambda) - 1 - 4\cos^2\frac{\mu}{4}$. We define

$$\begin{aligned}
D_1 &:= \{\lambda \notin \sigma_D | \quad D_s(\mu,\lambda) < 0, \quad D_c(\mu,\lambda) < 0\},\\
D_2 &:= \{\lambda \notin \sigma_D | \quad D_s(\mu,\lambda) < 0, \quad D_c(\mu,\lambda) > 0\},\\
D_3 &:= \{\lambda \notin \sigma_D | \quad D_s(\mu,\lambda) > 0, \quad D_c(\mu,\lambda) < 0\},\\
D_4 &:= \{\lambda \notin \sigma_D | \quad D_s(\mu,\lambda) > 0, \quad D_c(\mu,\lambda) > 0\}.
\end{aligned}$$

Putting

$$D_4^+ := \left\{\lambda \notin \sigma_D \middle| \quad d_c(\mu,\lambda) > 4\cos\frac{\mu}{4}, \quad d_s(\mu,\lambda) > 4\left|\sin\frac{\mu}{4}\right|\right\}$$

and

$$D_4^- := \left\{\lambda \notin \sigma_D \middle| \quad d_c(\mu,\lambda) < -4\cos\frac{\mu}{4}, \quad d_s(\mu,\lambda) < -4\left|\sin\frac{\mu}{4}\right|\right\},$$

we have the decomposition $D_4 = D_4^+ \cup D_4^-$. Then, we have the followings on the spectra of the fiber operator $H^\flat(\mu)$:

Theorem 2.1. *([4, Theorem 1.1])*
(0) For any $\mu \in S^1$, $\sigma_D \subset \sigma_p(H^\flat(\mu))$.
(1) If $\mu \in S^1 \setminus \{0\}$, then $D_1 \subset \sigma(H^\flat(\mu))$.
(2) If $\mu \in S^1 \setminus \{0\}$, then $D_2 \subset \sigma(H^\flat(\mu))$.
(3) If $\mu \in S^1 \setminus \{0, \pm\frac{2}{3}\pi\}$, then $D_3 \subset \sigma(H^\flat(\mu))$.
(4) If $\mu \in S^1 \setminus \{0, \pm\pi\}$, then $D_4^+ \subset \rho(H^\flat(\mu))$.

This theorem does not deal with D_4^-. The statements on the area D_4^- are more complicated. To state the corresponding statements, 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, we have the followings:

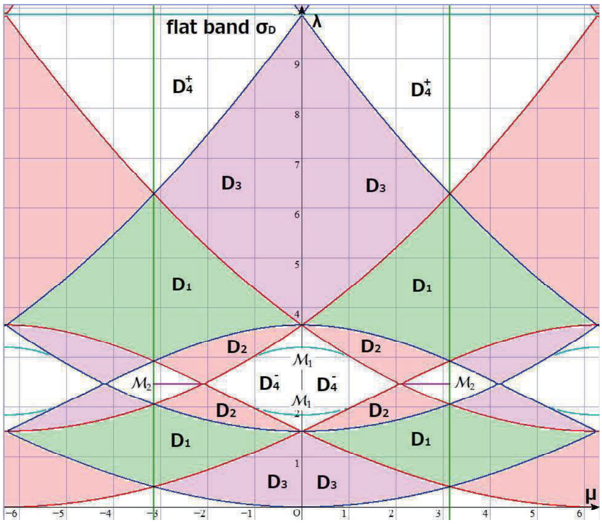

Figure 4: The dispersion relation for $q \equiv 0$.

Theorem 2.2. *([4, 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 $\theta_1 + 2\varphi_1' \neq 0$ *and* $3\Delta + \Delta_- = 0$.

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

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

(B) Assume that $\theta_1 + 2\varphi_1' \neq 0$ *and* $3\Delta + \Delta_- \neq 0$.

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

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

(C) Assume that $\theta_1 + 2\varphi_1' = 0$ *and q is even. If* $\frac{2}{3}\pi < |\mu| < \pi$, *then* $\lambda \in \sigma_p(H^\flat(\mu))$. *Otherwise,* $\lambda \in \rho(H^\flat(\mu))$.

(D) If $\theta_1 + 2\varphi_1' = 0$ *and q is not even, then* $\lambda \in \rho(H^\flat(\mu))$.

In the case of $q \equiv 0$, we see that $\theta_1 + 2\varphi_1' = 0$ and $3\Delta + \Delta_- = 0$ is equivalent. So, we derive only the results (B) and (C) for $q \equiv 0$. In order to understand the meaning of Theorems 2.1 and 2.2, we give the dispersion relation in the case of $q \equiv 0$. Let $\mathcal{M}_1$ and $\mathcal{M}_2$ be

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

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

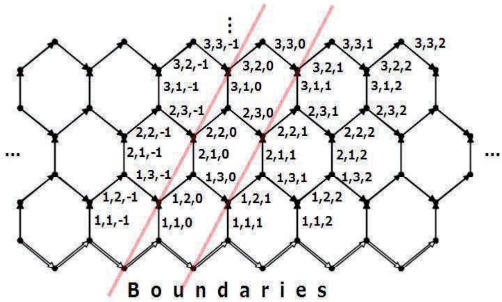

Figure 5: graphenes with zigzag boundary (without bumps)

where

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

and

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

Then, we derive a picture of the dispersion relation as seen in Fig. 4.

In order to compare the results for our quantum graph with the ones corresponding to graphene with standard zigzag boundaries discussed in [3]. Let $\Gamma^\sharp = (E^\sharp, V^\sharp)$ be the metric graph appearing in Fig. 5, where $E^\sharp$ and $V^\sharp$ are the set of edges and vertexes of $\Gamma^\sharp$, respectively. The difference between $\Gamma^\sharp$ and $\Gamma^\flat$ is whether or not the bumps are present. In a similar way to $H^\flat$, we assume that the length of each edge $e \in E^\sharp$ is equal to 1. For any $e \in E^\sharp$, the edge Hamiltonian $H^\sharp$ acts as

$$(H^\sharp y)_e(x) = -y_e''(x) + q(x)y_e(x), \quad x \in (0,1) \simeq e,$$

where the potential $q \in L^2(0,1)$ is the same one as $H^\flat$. Let the function $y \in \mathrm{Dom}(H^\sharp)$ be characterized the following two boundary conditions:

(a) the Kirchhoff vertex condition at any $v \in V^\sharp \setminus \partial\Gamma^\sharp$.

(b) the Dirichlet boundary condition $y \equiv 0$ on $\partial\Gamma^\sharp$.

Utilizing the periodicity of $\Gamma^\sharp$, we obtain the fiber operator $H^\sharp(\mu)$ to attain the unitarily equivalence

$$H^\sharp \simeq \int_{S^1}^{\oplus} H^\sharp(\mu) \frac{d\mu}{2\pi}.$$

Then, the function

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

for $\lambda \notin \sigma_D$ and $\mu \in S^1 \setminus \{\pm\pi\}$ plays the role of spectral discriminant for $H^\sharp$, where

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

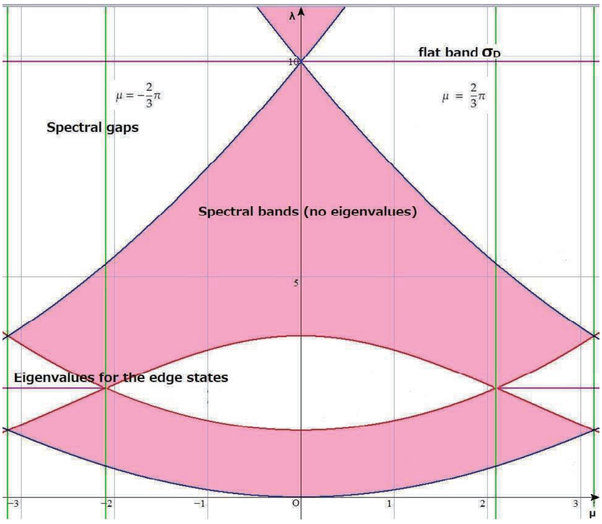

Figure 6: The dispersion relation for $q \equiv 0$.

Theorem 2.3. *([3, Thm 2.7.]) Assume that $\mu \in S^1 \setminus \{\pm\pi\}$.*
(0) $\sigma_D \subset \sigma(H^\sharp(\mu))$.
(1) Assume that $\lambda \notin \sigma_D$ and $D(\mu, \lambda) \leq 0$.

① *$\lambda \in \sigma(H^\sharp(\mu))$.*

② *If $D(\mu, \lambda) < 0$, then $\lambda \notin \sigma_p(H^\sharp(\mu))$.*

③ *If $D(\mu, \lambda) = 0$ and $\mu \neq \pm\frac{2}{3}\pi$, then $\lambda \notin \sigma_p(H^\sharp(\mu))$.*

(2) Assume that $\lambda \notin \sigma_D$ and $D(\mu, \lambda) > 0$.

① *If $\theta_1 + 2\varphi_1' \neq 0$, then $\lambda \in \rho(H^\sharp(\mu))$.*

② *If $\theta_1 + 2\varphi_1' = 0$ and $\mu \neq \pm\frac{2}{3}\pi$, then conditions*
(i) $\frac{2}{3}\pi < |\mu| < \pi$, (ii) $\lambda \in \sigma_p(H^\sharp(\mu))$, (iii) $\lambda \in \sigma(H^\sharp(\mu))$
are equivalent.

Based on Theorem 2.3, we derive a picture of the dispersion relation for $H^\sharp$. Compared Fig. 4 with Fig. 6, we find the eigenvalue line $\mathcal{M}_1$ in Fig. 4, which appears due to bumpy boundaries.

3 Outline of the proofs

The complete proofs of Theorems 2.1 and 2.2 are given in the original paper [4]. Thus, we give only an outline of the proof of Theorem 2.1 (2) here. Especially, we stress that a Key Tool to prove it is the Cramer's Rule in Linear Algebra:

Theorem 3.1. *Let* $\mathbf{a}_1, \mathbf{a}_2, \ldots, \mathbf{a}_n, \mathbf{b}, \mathbf{x} = (x_1, x_2, \ldots, x_n)^\top \in \mathbb{R}^n$ *and* $A = (\mathbf{a}_1 \quad \mathbf{a}_2 \quad \ldots \quad \mathbf{a}_n)$. *For a linear equation* $A\mathbf{x} = \mathbf{b}$, *we put*

$$A_i = (\mathbf{a}_1 \quad \cdots \quad \mathbf{a}_{i-1} \quad \mathbf{b} \quad \mathbf{a}_{i+1} \quad \cdots \quad \mathbf{a}_n).$$

If $\det A \neq 0$, *then we have*

$$x_i = \frac{\det A_i}{\det A}.$$

We utilize this theorem in the final phase of the proof of Theorem 2.1 (2). At first, we explain where the discriminants $D_s(\mu, \lambda)$ and $D_c(\mu, \lambda)$ are from. For a solution $y = (y_{n,j}) \in \mathrm{dom}(H^\flat(\mu))$ to $H^\flat(\mu)y = \lambda y$ on the fundamental domain $\Gamma_0^\flat$ (see Fig. 3), we define the 4×4 transfer matrix $M(\lambda) = (m_{ij}(\lambda))$ as

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

By straightforward calculations, we derive the components of $M(\lambda)$ and notice it has a block form:

Lemma 3.2. *Let* $\mu \in S^1 \setminus \{0\} = [-\pi, 0) \cup (0, \pi)$ *and* $\lambda \notin \sigma_D$. *Then, we have* $m_{11} = \frac{\theta_1'\varphi_1 + 2\Delta\theta_1}{1 - e^{-i\mu}}$ *and* $m_{12} = \frac{\varphi_1\varphi_1' + 2\Delta\varphi_1}{1 - e^{-i\mu}}$. *Furthermore, we obtain the block form*

$$M(\lambda) = \begin{pmatrix} A & e^{-i\mu}B \\ B & A \end{pmatrix}, \tag{3.1}$$

where

$$\begin{aligned} A &= \begin{pmatrix} m_{11} & m_{12} \\ \frac{2\Delta m_{11} - \theta_1}{\varphi_1} & -1 + \frac{2\Delta m_{12}}{\varphi_1} \end{pmatrix}, \\ B &= \begin{pmatrix} -m_{11} & -m_{12} \\ \frac{-2\Delta m_{11} - \theta_1 e^{i\mu}}{\varphi_1} & -e^{i\mu} - \frac{2\Delta m_{12}}{\varphi_1} \end{pmatrix}. \end{aligned}$$

With the help of the block form (3.1), we directly derive eigenvalues of the transfer matrix:

Lemma 3.3. *Assume that* $\mu \in S^1 \setminus \{0\}$ *and* $\lambda \notin \sigma_D$. *Then, the eigenvalues of* $M(\lambda)$ *are given by*

$$\rho_s^\pm = \frac{d_s(\mu,\lambda) \pm \sqrt{D_s(\mu,\lambda)}}{4ie^{-\frac{i\mu}{4}} \sin\frac{\mu}{4}}$$

and

$$\rho_c^\pm = \frac{d_c(\mu,\lambda) \pm \sqrt{D_c(\mu,\lambda)}}{4e^{-\frac{i\mu}{4}} \cos\frac{\mu}{4}}.$$

Put $S = \{\rho_s^+, \rho_s^-\} \cap \{\rho_c^+, \rho_c^-\}$. For the most part, each eigenvalue $\rho = \rho_s^\pm, \rho_c^\pm$ are simple:

Lemma 3.4.

(1) If $\mu \in S^1 \setminus \{0\}$, we have $S = \emptyset$ for almost every $\lambda \in D_1$.

(2) If $\mu \in S^1 \setminus \{0\}$, we have $S = \emptyset$ for every $\lambda \in D_2$.

(3) If $\mu \in S^1 \setminus \{0, \pm\frac{2}{3}\pi\}$, we have $S = \emptyset$ for every $\lambda \in D_3$.

(4) If $\mu \in S^1 \setminus \{0\}$, we have $S = \emptyset$ for every $\lambda \in D_4$.

Moreover, the eigenspace $V(\rho_c^\pm)$ and $V(\rho_s^\pm)$ can be explicitly written.

Lemma 3.5. *Assume that $\mu \in S^1 \setminus \{0\}$, $\lambda \notin \sigma_D$ 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[1].

These are spectral properties of the transfer matrix $M(\lambda)$. Next, we discuss the fundamental solutions to $H^\flat(\mu) = \lambda y$ for $\lambda \notin \sigma_D$. Taking the Kirchhoff vertex condition and the Dirichlet boundary condition into account, we have the following:

Lemma 3.6. *Let $\lambda \notin \sigma_D$ and $\mu \in S^1$. Then, any solution y to $H^\flat(\mu)y = \lambda y$ on $\Gamma_0^\flat$ 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 $y'_{0,2}(0, \lambda) = c_1 \in \mathbb{C}$.*

Thus, we construct the fundamental solutions $P = (p_{n,j})$ and $Q = (q_{n,j}) \in \mathrm{dom}(H^\flat(\mu))$ to $H^\flat(\mu)y = \lambda y$ with the initial conditions

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

respectively. For the purpose, we prepare notations. Let $P_c^\pm$ and $P_s^\pm$ be the projections to the eigenspace $V(\rho_c^\pm)$ and $V(\rho_s^\pm)$, respectively. Moreover, we hereafter assume that $\lambda \notin \sigma_D$, $\mu \in S^1 \setminus \{0\}$ and $\dim V(\rho_c^\pm) = \dim V(\rho_s^\pm) = 1$. Namely, we only consider (μ, λ) satisfying $S = \emptyset$ (see Lemma 3.4). 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 spectral decompositions

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

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

$$\mathbf{e}_{\ell,\bullet}^\pm = \begin{pmatrix} \alpha_{1,\ell,\bullet}^\pm & \beta_{1,\ell,\bullet}^\pm & \alpha_{4,\ell,\bullet}^\pm & \beta_{4,\ell,\bullet}^\pm \end{pmatrix}^\top.$$

[1] However, I avoid showing the explicit form here. See [4] for the explicit expression to $\mathbf{x}_c^\pm$ and $\mathbf{x}_s^\pm$.

We furthermore introduce $M_+(\lambda)$ and $M_-(\lambda)$ defined as follows:

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

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

In a similar way to the transfer matrix $M(\lambda)$, the components of $M_+(\lambda)$ and $M_-(\lambda)$ are explicitly written (see [4]). For $j = 2,3,5,6$, $\ell = 1,2$ and $\bullet = s,c$, we define $\alpha^{\pm}_{j,\ell,\bullet}$ and $\beta^{\pm}_{j,\ell,\bullet}$ by

$$\begin{pmatrix} \alpha^{\pm}_{2,\ell,\bullet} & \beta^{\pm}_{2,\ell,\bullet} & \alpha^{\pm}_{3,\ell,\bullet} & \beta^{\pm}_{3,\ell,\bullet} \end{pmatrix}^{\top} = M_+(\lambda)\mathbf{e}^{\pm}_{\ell,\bullet}, \tag{3.2}$$

$$\begin{pmatrix} \alpha^{\pm}_{5,\ell,\bullet} & \beta^{\pm}_{5,\ell,\bullet} & \alpha^{\pm}_{6,\ell,\bullet} & \beta^{\pm}_{6,\ell,\bullet} \end{pmatrix}^{\top} = M_-(\lambda)\mathbf{e}^{\pm}_{\ell,\bullet}. \tag{3.3}$$

We note that the values $\alpha^{\pm}_{j,\ell,\bullet}$ and $\beta^{\pm}_{j,\ell,\bullet}$ are defined for all $j = 1,2,3,4,5,6$, $\ell = 1,2$ and $\bullet = s,c$. Under these notations, we have he following:

Lemma 3.7. *Let $y = (y_{n,j})_{(n,j)\in\mathbb{Z}_0}$ be a solution to $H^{\flat}(\mu)y = \lambda y$ with*

$$\begin{pmatrix} y_{1,1}(0,\lambda) & y'_{1,1}(0,\lambda) & y_{1,4}(0,\lambda) & y'_{1,4}(0,\lambda) \end{pmatrix}^{\top} = c_1\mathbf{e}_1 + c_2\mathbf{e}_2.$$

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

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

where $\eta^{\pm}_{j,\ell,\bullet} = \eta^{\pm}_{j,\ell,\bullet}(x,\lambda) = \alpha^{\pm}_{j,\ell,\bullet}\theta(x,\lambda) + \beta^{\pm}_{j,\ell,\bullet}\varphi(x,\lambda)$ for $\ell = 1,2$ and $\bullet = s,c$.

For $(c_1,c_2) = (1,0)$, we have $y_{n,j}(x,\lambda) = p_{n,j}(x,\lambda)$. On the other hand, we have $y_{n,j}(x,\lambda) = q_{n,j}(x,\lambda)$ for $(c_1,c_2) = (0,1)$. Since the eigenvalues $\rho_s^{\pm}$ and $\rho_c^{\pm}$ are explicitly written, we make sure the following directly.

Lemma 3.8. *Assume that $\lambda \in D_2$ and $\mu \in S^1 \setminus \{0\}$. Then, $|\rho_s^{\pm}| = 1$, $|\rho_c^-| > 1$ and $|\rho_c^+| < 1$ hold true.*

Under these preparations, we give the proof of Theorem 2.2 (2).

Proof of Theorem 2.2 (2). Pick $\lambda \in D_2$, arbitrarily. We claim the following.

Claim: There exists some $(c_1,c_2) \neq (0,0)$ satisfying $c_1\eta^-_{j,1,s} + c_2\eta^-_{j,2,c} \equiv 0$ for all $j = 1,2,3,4,5,6$.

If this claim holds true, then $\|y_{n,j}\|_{L^2(0,1)}$ is uniformly bounded on $n \in \mathbb{N}$ and j. Since there exists a generalized eigenfunction to $H^{\flat}(\mu)y = \lambda y$, we have $\lambda \in \sigma(H^{\flat}(\mu))$.

To show the above claim, we want to find $(c_1, c_2) \neq (0,0)$ such that

$$c_1(\alpha^-_{j,1,c}\theta(x,\lambda) + \beta^-_{j,1,c}\varphi(x,\lambda)) + c_2(\alpha^-_{j,2,c}\theta(x,\lambda) + \beta^-_{j,2,c}\varphi(x,\lambda)) \equiv 0,$$

namely, $c_1\alpha^-_{j,1,c} + c_2\alpha^-_{j,2,c} = 0$ and $c_1\beta^-_{j,1,c} + c_2\beta^-_{j,2,c} = 0$ for any $j = 1,2,3,4,5,6$. Due to

$$\mathbf{e}^-_{1,c} = \begin{pmatrix} \alpha^-_{1,1,c} \\ \beta^-_{1,1,c} \\ \alpha^-_{4,1,c} \\ \beta^-_{4,1,c} \end{pmatrix} \quad \text{and} \quad \mathbf{e}^-_{2,c} = \begin{pmatrix} \alpha^-_{1,2,c} \\ \beta^-_{1,2,c} \\ \alpha^-_{4,2,c} \\ \beta^-_{4,2,c} \end{pmatrix},$$

let us find $(c_1, c_2) \neq (0,0)$ such that

$$c_1\mathbf{e}^-_{1,c} + c_2\mathbf{e}^-_{2,c} = \mathbf{o}$$

at first. Prepare another form of spectral decompositions

$$\begin{aligned} \mathbf{e}_1 &= \mathbf{e}^+_{1,c} + \mathbf{e}^-_{1,c} + \mathbf{e}^+_{1,s} + \mathbf{e}^-_{1,s} = \gamma^+_c\mathbf{w}^+_c + \gamma^-_c\mathbf{w}^-_c + \gamma^+_s\mathbf{w}^+_s + \gamma^-_s\mathbf{w}^-_s, \\ \mathbf{e}_2 &= \mathbf{e}^+_{2,c} + \mathbf{e}^-_{2,c} + \mathbf{e}^+_{2,s} + \mathbf{e}^-_{2,s} = \delta^+_c\mathbf{w}^+_c + \delta^-_c\mathbf{w}^-_c + \delta^+_s\mathbf{w}^+_s + \delta^-_s\mathbf{w}^-_s. \end{aligned}$$

Then, we want to find $(c_1, c_2) \neq (0,0)$ such that

$$c_1\gamma^-_c + c_2\delta^-_c = 0.$$

If $\gamma^-_c \neq 0$, then $(c_1, c_2) = (\delta^-_c, -\gamma^-_c)$ is the desired one.

To prove $\gamma^-_c \neq 0$, we utilize the Cramer's rule. The Cramer's rule yields

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

It follows by Lemma 3.4 that $\det(\mathbf{x}^+_c\ \mathbf{e}^+_1) \neq 0$. Putting

$$\mathbf{e}^+_1 = \begin{pmatrix} \varphi_1 \\ 2\Delta \end{pmatrix},$$

we have

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

Therefore, we derive $\gamma^-_c \neq 0$. Taking (3.2) and (3.3) into account, we also derive $\delta^-_c\alpha^-_{j,1,c} + (-\gamma^-_c)\alpha^-_{j,2,c} = 0$ and $\delta^-_c\beta^-_{j,1,c} + (-\gamma^-_c)\beta^-_{j,2,c} = 0$ for $j = 2,3,5,6$. □

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