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Spectral gaps of the one-dimensional Schrödinger operators with periodic point interactions

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Abstract. We study the spectral gaps of the Schrödinger operators

$$H_1 = -\frac{d^2}{dx^2} + \sum_{l=-\infty}^{\infty} \beta_1\delta'(x-\kappa-2\pi l) + \beta_2\delta'(x-2\pi l) \quad \text{in } L^2(\mathbb{R}),$$

$$H_2 = -\frac{d^2}{dx^2} + \sum_{l=-\infty}^{\infty} \beta_1\delta(x-\kappa-2\pi l) + \beta_2\delta(x-2\pi l) \quad \text{in } L^2(\mathbb{R}),$$

where $\kappa \in (0, 2\pi)$ and $\beta_1, \beta_2 \in \mathbb{R}\backslash\{0\}$ are parameters. Given $j \in \mathbb{N}$, we determine whether the jth gap of H_k is absent or not for $k = 1, 2$.

Key words: Schrödinger operators, periodic point interactions, spectral gaps.

1. Introduction

In this note we discuss the spectral gaps of the Schrödinger operators formally expressed as

$$H_1 = -\frac{d^2}{dx^2} + \sum_{l=-\infty}^{\infty} \big(\beta_1\delta'(x-\kappa-2\pi l) + \beta_2\delta'(x-2\pi l)\big) \quad \text{in } L^2(\mathbb{R}),$$

$$H_2 = -\frac{d^2}{dx^2} + \sum_{l=-\infty}^{\infty} \big(\beta_1\delta(x-\kappa-2\pi l) + \beta_2\delta(x-2\pi l)\big) \quad \text{in } L^2(\mathbb{R}),$$

where $\kappa \in (0, 2\pi)$ and $\beta_1, \beta_2 \in \mathbb{R}\backslash\{0\}$ are parameters, $\delta(x)$ stands for the Dirac delta function at the origin, and $\delta'(x)$ is the derivative of $\delta(x)$. The precise definitions of these operators are given through boundary conditions. Put

$$Z_1 = \{\kappa\} + 2\pi\mathbb{Z},\ Z_2 = 2\pi\mathbb{Z},\ Z = Z_1 \cup Z_2,$$

and

$$T_l^1 = \begin{pmatrix} 1 & \beta_l \\ 0 & 1 \end{pmatrix},\ T_l^2 = \begin{pmatrix} 1 & 0 \\ \beta_l & 1 \end{pmatrix} \quad \text{for} \quad l = 1, 2.$$

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For $k = 1, 2$, we define

$$(H_k y)(x) = -y''(x), \quad x \in \mathbb{R}\backslash Z,$$

$$\mathrm{Dom}(H_k) = \left\{ y \in H^2(\mathbb{R}\backslash Z) \,\middle|\, \begin{pmatrix} y(t+0) \\ y'(t+0) \end{pmatrix} = T_l^k \begin{pmatrix} y(t-0) \\ y'(t-0) \end{pmatrix} \quad \text{for} \quad t \in Z_l,\ l = 1, 2 \right\}.$$

It follows by [5, Theorem 3.1] that H_2 is self-adjoint. The proof of the self-adjointness of H_1 is similar to that of [5, Theorem 3.1].

Since the interactions are 2π-periodic, we can utilize the Floquet-Bloch reduction scheme (see [10, Section XIII.16]). For $\theta \in [0, 2\pi]$, we introduce the Hilbert space

$$\mathcal{H}_\theta = \{u \in L^2_{\mathrm{loc}}(\mathbb{R}) \mid u(x + 2\pi) = e^{\sqrt{-1}\theta} u(x) \quad \text{a.e.} \quad x \in \mathbb{R}\}$$

equipped with the inner product

$$(u,\, v)_{\mathcal{H}_\theta} = \int_0^{2\pi} u(x)\overline{v(x)}dx, \quad u,\, v \in \mathcal{H}_\theta.$$

We define the operator H_θ^k in $\mathcal{H}_\theta$ by

$$(H_\theta^k y)(x) = -y''(x), \quad x \in \mathbb{R}\backslash Z,$$

$$\mathrm{Dom}(H_\theta^k) = \left\{ y \in \mathcal{H}_\theta \,\middle|\, y \in H^2\big((0,\, 2\pi)\backslash\{\kappa\}\big), \begin{pmatrix} y(t+0) \\ y'(t+0) \end{pmatrix} = T_l^k \begin{pmatrix} y(t-0) \\ y'(t-0) \end{pmatrix} \quad \text{for} \quad t \in Z_l,\ l = 1,\, 2 \right\}.$$

We further introduce the unitary operator $\mathcal{U}$ from $L^2(\mathbb{R})$ onto $\int_0^{2\pi} \oplus \mathcal{H}_\theta d\theta$ defined as

$$(\mathcal{U}u)(x,\, \theta) = \frac{1}{\sqrt{2\pi}} \sum_{l=-\infty}^{\infty} e^{\sqrt{-1}l\theta} u(x - 2l\pi).$$

The operator H_k admits the direct integral representation

$$\mathcal{U} H_k \mathcal{U}^{-1} = \int_0^{2\pi} \oplus H_\theta^k d\theta.$$

For $\theta \in [0, 2\pi]$ and $j \in \mathbb{N} = \{1, 2, \ldots\}$, we denote by $\lambda_j^k(\theta)$ the jth eigenvalue of H_θ^k counted with multiplicity. The basic properties of $\lambda_j^k(\theta)$ and $\sigma(H_k)$ are summarized as follows.

Proposition 1 *The following claims hold true.*
(a) *The function* $\lambda_j^k(\,\cdot\,)$ *is continuous on* $[0, 2\pi]$.
(b) *We have* $\lambda_j^k(\theta) = \lambda_j^k(2\pi - \theta)$.
(c) *For* $\theta \in (0, \pi)$, *all the eigenvalues of* H_θ^k *are simple.*
(d) *If* $\beta_1\beta_2 > 0$ *or* $k = 2$, *then the function* $\lambda_j^k(\theta)$ *is strictly monotone increasing* (*respectively, decreasing*) *as* θ *varies from* 0 *to* π *for odd* (*respectively, even*) j.
(e) *If* $\beta_1\beta_2 < 0$ *and* $k = 1$, *then the function* $\lambda_j^k(\theta)$ *is strictly monotone decreasing* (*respectively, increasing*) *as* θ *varies from* 0 *to* π *for odd* (*respectively, even*) j.
(f) *The spectrum of* H_k *is expressed as*

$$\begin{aligned}\sigma(H_k) &= \bigcup_{j=1}^{\infty} \lambda_j^k([0, \pi]) \\ &= \bigcup_{j=1}^{\infty} \bigcup_{\theta \in [0, \pi]} \{\lambda_j^k(\theta)\}.\end{aligned}$$

We define

$$G_j^k = \begin{cases} \big(\lambda_j^k(\pi), \lambda_{j+1}^k(\pi)\big) & \text{for } j \text{ odd,} \\ \big(\lambda_j^k(0), \lambda_{j+1}^k(0)\big) & \text{for } j \text{ even} \end{cases}$$

in the case that $k = 2$ or $\beta_1\beta_2 > 0$, while we set

$$G_j^k = \begin{cases} \big(\lambda_j^k(\pi), \lambda_{j+1}^k(\pi)\big) & \text{for } j \text{ even,} \\ \big(\lambda_j^k(0), \lambda_{j+1}^k(0)\big) & \text{for } j \text{ odd} \end{cases}$$

if $k = 1$ and $\beta_1\beta_2 < 0$. We also put

$$B_j^k = \lambda_j^k([0, \pi]).$$

The closed interval B_j^k is called the jth band of the spectrum of H_k, the open interval G_j^k the jth gap. The purpose of this note is to determine whether the jth gap is empty or not for a given $j \in \mathbb{N}$. Our main results are the following two theorems.

Theorem 2 *Suppose $\beta_1 \neq \beta_2$ and $\beta_1 + \beta_2 \neq -2\pi$.*
(i) *If either $\beta_1 + \beta_2 \neq 0$ or $\kappa/\pi \notin \mathbb{Q}$ holds, then we have*

$$G_j^1 \neq \emptyset \quad for \quad j \in \mathbb{N}.$$

(ii) *Let $\beta_1 + \beta_2 = 0$, $\kappa/\pi = m/n$, $(m, n) \in \mathbb{N}^2$, $\gcd(m, n) = 1$, and $m \notin 2\mathbb{N}$. Then we have*

$$G_j^1 = \emptyset \quad if \quad j - 1 \in 2n\mathbb{N},$$
$$G_j^1 \neq \emptyset \quad if \quad j - 1 \notin 2n\mathbb{N}.$$

(iii) *If $\beta_1+\beta_2 = 0$, $\kappa/\pi = m/n$, $(m, n) \in \mathbb{N}^2$, $\gcd(m, n) = 1$, and $m \in 2\mathbb{N}$, then we have*

$$G_j^1 = \emptyset \quad for \quad j - 1 \in n\mathbb{N},$$
$$G_j^1 \neq \emptyset \quad for \quad j - 1 \notin n\mathbb{N}.$$

Theorem 3 *Assume $\beta_1 \neq \beta_2$.*
(i) *If either $\beta_1 + \beta_2 \neq 0$ or $\kappa/\pi \notin \mathbb{Q}$ holds, then we have*

$$G_j^2 \neq \emptyset \quad for \quad j \in \mathbb{N}.$$

(ii) *If $\beta_1 + \beta_2 = 0$, $\kappa/\pi = m/n$, $(m, n) \in \mathbb{N}^2$, $\gcd(m, n) = 1$ and $m \notin 2\mathbb{N}$, then we have*

$$G_j^2 = \emptyset \quad for \quad j \in 2n\mathbb{N},$$
$$G_j^2 \neq \emptyset \quad for \quad j \notin 2n\mathbb{N}.$$

(iii) *Let $\beta_1 + \beta_2 = 0$, $\kappa/\pi = m/n$, $(m, n) \in \mathbb{N}^2$, $\gcd(m, n) = 1$ and $m \in 2\mathbb{N}$. Then we have*

$$G_j^2 = \emptyset \quad if \quad j \in n\mathbb{N},$$
$$G_j^2 \neq \emptyset \quad if \quad j \notin n\mathbb{N}.$$

The one-dimensional Schrödinger operators with periodic point interactions have been studied by numerous authors; we refer to [3, 4, 6, 8] and [1, 2] for a thorough review. R. Kronig and W. Penney were the first to introduce such an operator; they studied in [8] the spectrum of the operator $L_1 = -d^2/dx^2 + \alpha \sum_{l=-\infty}^{\infty} \delta(x - al)$ in $L^2(\mathbb{R})$, where $\alpha \in \mathbb{R}\backslash\{0\}$ and $a > 0$ are constants. This operator, which is called the Kronig-Penney Hamiltonian, serves as the most fundamental model in the modern textbooks of solid-state physics (see e.g. [7]). The Kronig-Penney Hamiltonian was extensively generalized with the advance of the theory of point interactions. In [3, 4] F. Gesztesy, H. Holden, and W. Kirsch introduced the operator $L_2 = -d^2/dx^2 + \alpha\sum_{l=-\infty}^{\infty}\delta'(x-al)$ in $L^2(\mathbb{R})$ and discussed its spectral properties in detail. Among other results they prove that every gap of $\sigma(L_2)$ is present if $\alpha \neq -a$ and that only the first gap is absent if $\alpha = -a$. In [4] it is also showed that every gap of $\sigma(L_1)$ is present. In [6] R. Hughes performed the Floquet analysis on the following operator which involved the generalized point interaction:

$$(L_3 y)(x) = -y''(x), \quad x \in \mathbb{R}\backslash a\mathbb{Z},$$

$$\mathrm{Dom}(L_3) = \left\{ y \in H^2(\mathbb{R}\backslash a\mathbb{Z}) \;\middle|\; \begin{pmatrix} y(aj+0) \\ y'(aj+0) \end{pmatrix} = cA \begin{pmatrix} y(aj-0) \\ y'(aj-0) \end{pmatrix}, \quad j \in \mathbb{Z} \right\},$$

where $A \in \mathrm{SL}_2(\mathbb{R})$, $c \in \mathbb{C}$, and $|c| = 1$. It is also proved in [6] that all the gaps of $\sigma(L_3)$ are absent in the case that $c = 1$ and $A = -I$, where I stands for the 2×2 identity matrix. We further recall the well-known fact that every gap of the spectrum of the Mathieu operator $-d^2/dx^2 + \alpha\cos(2\pi x/a)$ in $L^2(\mathbb{R})$ is present (see [10, Section XIII.16, Example 1] and [9, Section 7] for related topics).

In most works on the one-dimensional Schrödinger operators with periodic point interactions, the interaction support is supposed to be identically spaced lattice $a\mathbb{Z}$. On the contrast, this paper is based on an interest in the interactions supported on the non-identically spaced lattice $\{0, \kappa\} + 2\pi\mathbb{Z}$. Our main results say that some gaps of the spectrum of L_2 (respectively, L_1) begin to be absent when the second interaction $-\alpha\sum_{l=-\infty}^{\infty}\delta'(x-s-al)$ (respectively, $-\alpha\sum_{l=-\infty}^{\infty}\delta(x-s-al)$) with $s/a \in \mathbb{Q}\backslash\mathbb{Z}$ is turned on it.

The next section is devoted to the proof of the results. Since the proof of the assertion for $\sigma(H_2)$ is similar to that for $\sigma(H_1)$, we demonstrate only Theorem 2 and Proposition 1 for $k = 1$. Let us review our idea in proving Theorem 2. The band edges are given by the zeros of the function $D(\,\cdot\,) \pm 2$, where D is the discriminant defined by (4). Although the discriminant is expressed in an explicit way in terms of κ and λ, the double zeros of $D(\,\cdot\,) \pm 2$ is somewhat hard to discuss directly because of the complexity of the expression of this function. We eliminate this difficulty by using the monodromy matrix; we reduce the problem to a system of algebraic equations (9) $\sim$ (11) in the proof of Lemma 5, which is a key lemma in proving Theorem 2. We remark that the assumptions $\beta_1 \neq \beta_2$ and $\beta_1 + \beta_2 \neq -2\pi$ in Theorem 2 are essential; it can be showed that if $\beta_1 + \beta_2 = -2\pi$, then one of the gaps of $\sigma(H_1)$ disappears at the origin.

2. Proof of the results

Let us consider the equation

$$\begin{cases} -y''(x) = \lambda y(x) & \text{on} \quad \mathbb{R}\backslash Z, \\ \begin{pmatrix} y(t+0) \\ y'(t+0) \end{pmatrix} = \begin{pmatrix} 1 & \beta_l \\ 0 & 1 \end{pmatrix} \begin{pmatrix} y(t-0) \\ y'(t-0) \end{pmatrix} & \text{for} \quad t \in Z_l,\ l = 1,\, 2, \end{cases} \tag{1}$$

where λ is a real parameter. By $y_1(x, \lambda)$ and $y_2(x, \lambda)$ we denote the solutions of this equation subject to the initial conditions

$$\big(y_1(+0, \lambda),\, y_1'(+0, \lambda)\big) = (1,\, 0) \tag{2}$$

and

$$\big(y_2(+0, \lambda),\, y_2'(+0, \lambda)\big) = (0,\, 1), \tag{3}$$

respectively. Let $D(\lambda)$ be the discriminant of the equation (1):

$$D(\lambda) = y_1(2\pi + 0,\, \lambda) + y_2'(2\pi + 0,\, \lambda). \tag{4}$$

The sequence $\{\lambda_j^1(0)\}_{j=1}^{\infty}$ gives all the zeros of the function $D(\,\cdot\,)-2$ counted with multiplicity, while the sequence $\{\lambda_j^1(\pi)\}_{j=1}^{\infty}$ provides all the zeros of the function $D(\,\cdot\,)+2$ repeated according to multiplicity. We further introduce the monodromy matrix of (1):

$$M(\lambda) = \begin{pmatrix} m_{11}(\lambda) & m_{12}(\lambda) \\ m_{21}(\lambda) & m_{22}(\lambda) \end{pmatrix} = \begin{pmatrix} y_1(2\pi + 0,\, \lambda) & y_2(2\pi + 0,\, \lambda) \\ y_1'(2\pi + 0,\, \lambda) & y_2'(2\pi + 0,\, \lambda) \end{pmatrix}.$$

Put $\tau = 2\pi - \kappa$. By a straightforward computation, we obtain

$$\begin{aligned} m_{11}(\lambda) = {} & \cos\tau\sqrt{\lambda}\cos\kappa\sqrt{\lambda} \\ & - (\beta_1 + \beta_2)\sqrt{\lambda}\cos\tau\sqrt{\lambda}\sin\kappa\sqrt{\lambda} \\ & - \beta_2\sqrt{\lambda}\sin\tau\sqrt{\lambda}\cos\kappa\sqrt{\lambda} \\ & + (\beta_1\beta_2\lambda - 1)\sin\tau\sqrt{\lambda}\sin\kappa\sqrt{\lambda}, \end{aligned} \tag{5}$$

$$\begin{aligned}
m_{12}(\lambda) = &(\beta_1 + \beta_2)\cos\tau\sqrt{\lambda}\cos\kappa\sqrt{\lambda} \\
&+ \Big(\frac{1}{\sqrt{\lambda}} - \beta_1\beta_2\sqrt{\lambda}\Big)\sin\tau\sqrt{\lambda}\cos\kappa\sqrt{\lambda} \\
&+ \frac{1}{\sqrt{\lambda}}\cos\tau\sqrt{\lambda}\sin\kappa\sqrt{\lambda} - \beta_2\sin\tau\sqrt{\lambda}\sin\kappa\sqrt{\lambda}, \qquad (6) \\
m_{21}(\lambda) = &-\sqrt{\lambda}\sin\tau\sqrt{\lambda}\cos\kappa\sqrt{\lambda} + \beta_1\lambda\sin\tau\sqrt{\lambda}\sin\kappa\sqrt{\lambda} \\
&- \sqrt{\lambda}\cos\tau\sqrt{\lambda}\sin\kappa\sqrt{\lambda}, \qquad (7) \\
m_{22}(\lambda) = &\cos\tau\sqrt{\lambda}\cos\kappa\sqrt{\lambda} - \beta_1\sqrt{\lambda}\sin\tau\sqrt{\lambda}\cos\kappa\sqrt{\lambda} \\
&- \sin\tau\sqrt{\lambda}\sin\kappa\sqrt{\lambda} \qquad (8)
\end{aligned}$$

for $\lambda \neq 0$, where we fix the branch of the square root as

$$\arg\sqrt{\lambda} \in \Big\{0,\ \frac{\pi}{2}\Big\}$$

for the sake of definiteness. Besides, we have

$$m_{11}(0) = 1, \quad m_{12}(0) = \beta_1 + \beta_2 + 2\pi, \quad m_{21}(0) = 0, \quad m_{22}(0) = 1.$$

First, we prove the following implication.

Lemma 4 *We have $M(\lambda) = I$ (respectively, $M(\lambda) = -I$) if and only if λ is a double eigenvalue of H_0^1 (respectively, H_π^1).*

Proof. Assume that λ is a double eigenvalue of H_0^1. Let $\{w_1(x),\, w_2(x)\}$ be a basis of $\mathrm{Ker}(H_0^1 - \lambda)$. Since $w_1(x)$ and $w_2(x)$ are linearly independent solutions of (1), we see that $y_1(x)$ and $y_2(x)$ are linear combinations of $w_1(x)$ and $w_2(x)$. Thus we get $y_1, y_2 \in \mathrm{Dom}(H_0^1)$. This together with (2) and (3) implies $M(\lambda) = I$.

Next we prove the converse. Assume that $M(\lambda) = I$. This combined with (2) and (3) yields $y_1,\, y_2 \in \mathrm{Dom}(H_0^1)$. Since $y_1(x)$ and $y_2(x)$ solve the equation (1), we have $y_1,\, y_2 \in \mathrm{Ker}(H_0^1 - \lambda)$. Since y_1 and y_2 are linearly independent, we infer that λ is a double eigenvalue of H_0^1.

In a similar way, we claim that $M(\lambda) = -I$ if and only if λ is a double eigenvalue of H_π^1. □

To prove Theorem 2 we need the assumption

(A.1) $\beta_1 \neq \beta_2$ and $\beta_1 + \beta_2 \neq -2\pi$.

The following lemma plays the most important role in the demonstration of Theorem 2.

Lemma 5 *Suppose* (A.1). *If* $M(\lambda) = I$ *or* $M(\lambda) = -I$, *then we have* $\sin\tau\sqrt{\lambda} = \sin\kappa\sqrt{\lambda} = 0$, $\lambda \neq 0$, *and* $\beta_1 + \beta_2 = 0$.

Proof. Suppose that $M(\lambda) = I$ or $M(\lambda) = -I$. First, we prove that $\sin\tau\sqrt{\lambda}\sin\kappa\sqrt{\lambda} = 0$. Seeking a contradiction, we assume that

$$\sin\tau\sqrt{\lambda}\sin\kappa\sqrt{\lambda} \neq 0.$$

We define $x_1 = \cot\kappa\sqrt{\lambda}$, $x_2 = \cot\tau\sqrt{\lambda}$, and $C_l = \beta_l\sqrt{\lambda}$ for $l = 1, 2$. Inserting (5) $\sim$ (8) into the equalities

$$m_{11}(\lambda) - m_{22}(\lambda) = 0,$$
$$\sqrt{\lambda}m_{12}(\lambda) = 0,$$
$$\frac{1}{\sqrt{\lambda}}m_{21}(\lambda) = 0,$$

and dividing those by $\sin\tau\sqrt{\lambda}\sin\kappa\sqrt{\lambda}$, we have

$$(C_1 - C_2)x_1 - (C_1 + C_2)x_2 + C_1C_2 = 0, \tag{9}$$
$$(C_1 + C_2)x_2x_1 + (1 - C_1C_2)x_1 + x_2 - C_2 = 0, \tag{10}$$
$$-x_1 - x_2 + C_1 = 0, \tag{11}$$

respectively. Using (9), (11), and $C_1 \neq 0$, we get

$$x_1 = x_2 = \frac{C_1}{2}. \tag{12}$$

Plugging this into (10), we infer that

$$(C_1 - C_2)\Big(\frac{1}{4}C_1^2 + 1\Big) = 0.$$

Since $\beta_1 \neq \beta_2$ and $\lambda \neq 0$, we have $C_1 - C_2 \neq 0$ and hence $C_1^2 = -4$. By (12) we arrive at

$$x_1 = x_2 = \pm\sqrt{-1}.$$

However, this violates the fact that $\cot z \neq \pm\sqrt{-1}$ for all $z \in \mathbb{C}$. Hence we have

$$\sin\tau\sqrt{\lambda}\sin\kappa\sqrt{\lambda} = 0,$$

namely,

$$\sin \tau\sqrt{\lambda} = 0 \quad \text{or} \quad \sin \kappa\sqrt{\lambda} = 0. \tag{13}$$

Next we prove that $\lambda \neq 0$. Since $\beta_1 + \beta_2 \neq -2\pi$ by assumption, we have

$$m_{12}(0) = 2\pi + \beta_1 + \beta_2 \neq 0.$$

This together with $m_{12}(\lambda) = 0$ implies that $\lambda \neq 0$.

In the former case of (13), we claim by $m_{21}(\lambda) = 0$ and (7) that

$$m_{21}(\lambda) = -\sqrt{\lambda}\cos \tau\sqrt{\lambda}\sin \kappa\sqrt{\lambda} = 0$$

and thus $\sin \kappa\sqrt{\lambda} = 0$. In the latter case of (13), we infer by (5), (8), and $m_{11}(\lambda) - m_{22}(\lambda) = 0$ that

$$m_{11}(\lambda) - m_{22}(\lambda) = (\beta_1 - \beta_2)\sqrt{\lambda}\sin \tau\sqrt{\lambda}\cos \kappa\sqrt{\lambda} = 0$$

and hence $\sin \tau\sqrt{\lambda} = 0$. Therefore, we get

$$\sin \tau\sqrt{\lambda} = \sin \kappa\sqrt{\lambda} = 0$$

in each case of (13). Combining this with $m_{12}(\lambda) = 0$ and (6), we get

$$m_{12}(\lambda) = (\beta_1 + \beta_2)\cos \tau\sqrt{\lambda}\cos \kappa\sqrt{\lambda} = 0$$

and thus $\beta_1 + \beta_2 = 0$. □

We prove Proposition 1 at the very end of this section. Assuming this fact for the moment, we complete the proof of Theorem 2.

Proof of Theorem 2 (i). Since $\{z \in \mathbb{C} \mid \sin z = 0\} = \pi\mathbb{Z}$ and since $\tau = 2\pi - \kappa$, we infer that the following two statements are equivalent.

- There exists $\lambda \neq 0$ such that $\sin \tau\sqrt{\lambda} = \sin \kappa\sqrt{\lambda} = 0$.
- $\kappa \in \pi\mathbb{Q}$.

This together with Lemma 5 and Proposition 1 yields the conclusion. □

Next we turn to the proofs of Theorem 2 (ii) and (iii). We assume

(A.2) $\beta_1 + \beta_2 = 0$, $\kappa/\pi = m/n$, $(m, n) \in \mathbb{N}^2$, and $\gcd(m, n) = 1$.

The following lemma provides the double eigenvalues of H_0^1 or H_π^1.

Lemma 6 *Suppose* (A.2)*. If* $m \notin 2\mathbb{N}$*, then we have*

$$\{\lambda \in \mathbb{R} \mid M(\lambda) = I \quad or \quad M(\lambda) = -I\} = \{j^2 n^2 \mid j \in \mathbb{N}\}. \tag{14}$$

If $m \in 2\mathbb{N}$*, then we get*

$$\{\lambda \in \mathbb{R} \mid M(\lambda) = I \quad or \quad M(\lambda) = -I\} = \left\{\frac{j^2 n^2}{4} \;\middle|\; j \in \mathbb{N}\right\}. \tag{15}$$

Proof. First, we discuss the case that $m \notin 2\mathbb{N}$. Suppose that $M(\lambda) = I$ or $M(\lambda) = -I$. Then we infer by Lemma 5 that $\sin\tau\sqrt{\lambda} = \sin\kappa\sqrt{\lambda} = 0$ and $\lambda \neq 0$. Combining this with $\tau = 2\pi - \kappa$, $\kappa/\pi = m/n$, $(m, n) \in \mathbb{N}^2$, $\gcd(m, n) = 1$, and $m \notin 2\mathbb{N}$, we infer that there exists a $j \in \mathbb{N}$ for which $\lambda = n^2 j^2$. On the other hand, we claim by (5) $\sim$ (8) that $M(n^2 i^2) = I$ for $i \in \mathbb{N}$. Hence, we obtain (14). The proof of (15) is similar. □

Let us demonstrate the following claim.

Lemma 7 *Suppose* (A.2) *and* $j \in \mathbb{N} \cup \{0\}$*. If* $m \notin 2\mathbb{N}$*, then the function* $D(\cdot)$ *admits exactly* $2n$ *zeros inside the interval* $(n^2 j^2, n^2(j+1)^2)$*. If* $m \in 2\mathbb{N}$*, then the function* $D(\cdot)$ *has exactly* n *zeros inside the interval* $(n^2 j^2/4, n^2(j+1)^2/4)$*.*

Proof. Since $\beta_1 + \beta_2 = 0$, we have

$$\begin{aligned} D(\lambda) &= 2\cos\tau\sqrt{\lambda}\cos\kappa\sqrt{\lambda} - (\beta_1^2\lambda + 2)\sin\tau\sqrt{\lambda}\sin\kappa\sqrt{\lambda} \\ &= \sqrt{\beta_1^2\lambda + 2}\sin\tau\sqrt{\lambda}\cos\kappa\sqrt{\lambda} \\ &\quad \times \left(\frac{2}{\sqrt{\beta_1^2\lambda + 2}}\cot\tau\sqrt{\lambda} - \sqrt{\beta_1^2\lambda + 2}\tan\kappa\sqrt{\lambda}\right). \end{aligned} \tag{16}$$

We fix $j \in \mathbb{N} \cup \{0\}$. First, we demonstrate the assertion for $m \notin 2\mathbb{N}$. We define

$$\begin{aligned} &f_1(\lambda) = \sqrt{\beta_1^2\lambda + 2}\tan\kappa\sqrt{\lambda}, \quad f_2(\lambda) = \frac{2}{\sqrt{\beta_1^2\lambda + 2}}\cot\tau\sqrt{\lambda}, \\ &P_1 = \left\{\lambda \in (n^2 j^2, n^2(j+1)^2) \;\middle|\; \kappa\sqrt{\lambda} \in \left\{\frac{\pi}{2}\right\} + \pi\mathbb{Z}\right\}, \\ &P_2 = \{\lambda \in (n^2 j^2, n^2(j+1)^2) \mid \tau\sqrt{\lambda} \in \pi\mathbb{Z}\}, \\ &P = P_1 \cup P_2, \\ &S = \{\lambda \in (n^2 j^2, n^2(j+1)^2) \mid D(\lambda) = 0\}, \\ &S_1 = \{\lambda \in (n^2 j^2, n^2(j+1)^2)\backslash P \mid f_1(\lambda) = f_2(\lambda)\}, \end{aligned}$$

$$S_2 = \{\lambda \in (n^2 j^2,\, n^2(j+1)^2) \mid \sin \tau\sqrt{\lambda} = \cos \kappa\sqrt{\lambda} = 0\}.$$

By (16) we have

$$S = S_1 \cup S_2.$$

Put

$$q_{1,k} = \left(\frac{1}{\kappa}\Big(mj\pi + \frac{\pi}{2}(2k-1)\Big)\right)^2 \quad \text{for} \quad k = 1,\, 2,\, \ldots,\, m,$$

$$q_{2,l} = \left(\frac{1}{\tau}\big((2n-m)j\pi + l\pi\big)\right)^2 \quad \text{for} \quad l = 1,\, 2,\, \ldots,\, 2n-m-1,$$

$$r = \sharp\{(k,\, l) \in \mathbb{N}^2 \mid k \le m,\, l \le 2n-2m-1,\, q_{1,k} = q_{2,l}\}.$$

We obtain

$$P_1 = \bigcup_{k=1}^{m} \{q_{1,k}\}, \quad P_2 = \bigcup_{l=1}^{2n-m-1} \{q_{2,l}\},$$

$$\sharp S_2 = r, \quad \sharp P = 2n - r - 1.$$

Let $\{r_s\}_{s=1}^{2n-r-1}$ be the rearrangement of the elements of P such that $r_s < r_{s+1}$ for $s = 1,\, 2,\, \ldots,\, 2n-r-2$. We define $r_0 = q_{2,0} = n^2 j^2$ and $r_{2n-r} = q_{2,\,2n-m} = n^2(j+1)^2$. Notice that

$$f_1(\lambda) \to \mp\infty \quad \text{as} \quad \lambda \to q_{1,k} \pm 0 \quad \text{for} \quad k = 1,\, 2,\, \ldots,\, m,$$

$$f_2(\lambda) \to \pm\infty \quad \text{as} \quad \lambda \to q_{2,l} \pm 0 \quad \text{for} \quad l = 0,\, 1,\, \ldots,\, 2n-m,$$

and that the function $f_s(\lambda)$ is continuous on $(n^2 j^2,\, n^2(j+1)^2)\backslash P_s$ for $s = 1,\, 2$. Furthermore, we have

$$\begin{aligned} f_1'(\lambda) &= \frac{1}{2\sqrt{\beta_1^2\lambda + 2\cos^2 \kappa\sqrt{\lambda}}}\Big(\frac{1}{2}\beta_1^2 \sin 2\kappa\sqrt{\lambda} + \beta_1^2\kappa\sqrt{\lambda} + \frac{2\kappa}{\sqrt{\lambda}}\Big) \\ &\ge \frac{\kappa}{\sqrt{\lambda}\sqrt{\beta_1^2\lambda + 2\cos^2 \kappa\sqrt{\lambda}}} \\ &> 0 \end{aligned}$$

on $(n^2 j^2,\, n^2(j+1)^2)\backslash P_1$, because $\sin t + t \ge 0$ for $t \ge 0$. Likewise, we get $f_2'(\lambda) < 0$ on $(n^2 j^2,\, n^2(j+1)^2)\backslash P_2$. Thus, we infer that the equation $f_1(\lambda) = f_2(\lambda)$ admits exactly one root on $(r_s,\, r_{s+1})$ for each $s = 0,\, 1,\, \ldots,\, 2n-r-1$. So we get $\sharp S_1 = 2n - r$ and hence $\sharp S = 2n$. Therefore we get the assertion for $m \notin 2\mathbb{N}$. In a similar way, we get the conslusion for $m \in 2\mathbb{N}$. □

We further need the following implication.

Lemma 8 *Suppose* (A.2)*. The function* $D(\,\cdot\,)$ *admits a unique zero in the interval* $(-\infty, 0]$*.*

Proof. Put

$$h_1(\lambda) = \frac{2}{\beta_1^2\lambda + 2}, \quad h_2(\lambda) = -\tanh\tau\sqrt{-\lambda}\tanh\kappa\sqrt{-\lambda} \quad \text{for } \lambda \le 0.$$

By (16) we have

$$\begin{aligned} D(\lambda) &= \cos\tau\sqrt{\lambda}\cos\kappa\sqrt{\lambda}\big(2-(\beta_1^2\lambda+2)\tan\tau\sqrt{\lambda}\tan\kappa\sqrt{\lambda}\big) \\ &= (\beta_1^2\lambda+2)\cos\tau\sqrt{\lambda}\cos\kappa\sqrt{\lambda}\big(h_1(\lambda)-h_2(\lambda)\big). \end{aligned}$$

Note that $h_2(\lambda)$ is a continuous, non-positive, strictly monotone increasing function on $(-\infty, 0]$. Note also that $h_1(\lambda)$ is a continuous function on $(-\infty, -2/\beta_1^2) \cup (-2/\beta_1^2, 0]$ and that

$$h_1'(\lambda) < 0 \quad \text{on} \quad \Big(-\infty, -\frac{2}{\beta_1^2}\Big) \cup \Big(-\frac{2}{\beta_1^2}, 0\Big],$$

$$\lim_{\lambda\to-\infty} h_1(\lambda) = 0, \qquad \lim_{\lambda\to-2/\beta_1^2-0} h_1(\lambda) = -\infty,$$

$$h_1(\lambda) > 0 \quad \text{on} \quad \Big(-\frac{2}{\beta_1^2}, 0\Big].$$

Thus the equation $h_1(\lambda) = h_2(\lambda)$ admits a unique root on $(-\infty, -2/\beta_1^2)$ and has no root on $(-2/\beta_1^2, 0]$. This together with $D(-2/\beta_1^2) \neq 0$ yields the conclusion. □

Now we are ready to prove (ii) and (iii) of Theorem 2.

Proof of Theorem 2 (ii), (iii). Note that all the zeros of $D(\cdot)$ are given by the sequence $\{\lambda_j^1(\pi/2)\}_{j=1}^{\infty}$ and that $\beta_1\beta_2 < 0$. This together with Proposition 1 and Lemmas 6, 7, and 8 implies the assertions. □

While the proof of Proposition 1 is almost same as those of [10, Theorems XIII.89 and XIII.90], we demonstrate this proposition for the sake of completeness.

Proof of Proposition 1. Now we suppose only $\beta_1, \beta_2 \in \mathbb{R}\backslash\{0\}$. A subtlety arises only in (d) and (e). First we discuss (e). Suppose $\beta_1\beta_2 < 0$. By (4), (5), and (8) we have

$$\lim_{\lambda\to-\infty} D(\lambda) = -\infty. \tag{17}$$

Note that λ is an eigenvalue of H^1_θ if and only if $D(\lambda) = 2\cos\theta$. This combined with (17) implies that

$$D(\lambda) < -2 \quad \text{for} \quad \lambda < \lambda^1_1(\pi), \tag{18}$$

$$\lambda^1_1(\theta) \geq \lambda^1_1(\pi) \quad \text{for} \quad \theta \in [0,\, \pi]. \tag{19}$$

Let us prove that $\lambda^1_1(\pi)$ is a simple eigenvalue. Seeking a contradiction, we assume that $\lambda^1_1(\pi)$ is a double eigenvalue. Since

$$D(\lambda^1_j(\theta)) = 2\cos\theta \quad \text{for} \quad \theta \in [0,\, \pi] \text{ and } j \in \mathbb{N}, \tag{20}$$

we claim by (19) that

$$\lambda^1_1\Big(\frac{\pi}{2}\Big) > \lambda^1_1(\pi) = \lambda^1_2(\pi). \tag{21}$$

By (c) we have

$$\lambda^1_1\Big(\frac{\pi}{2}\Big) < \lambda^1_2\Big(\frac{\pi}{2}\Big).$$

This combined with (21) and (a) implies that there exists a $\theta_0 \in (\pi/2,\, \pi)$ for which

$$\lambda^1_2(\theta_0) = \lambda^1_1\Big(\frac{\pi}{2}\Big).$$

However, this violates (20). So we conclude that $\lambda^1_1(\pi)$ is a simple eigenvalue. Thus we get the assertion in (e) by mimicking the arguments in the proof of [10, TheoremXIII.89(e)], (see also the proof of [6, Theorem 2]). We also obtain the claim in (d) by noticing

$$\lim_{\lambda\to-\infty} D(\lambda) = +\infty \quad \text{if} \quad \beta_1\beta_2 > 0.$$

□

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