On the Spectra of Schrödinger Operators on Zigzag Nanotubes with Multiple Bonds

By

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Abstract. In this paper, we study the spectral structure of periodic Schrödinger operators on a generalization of carbon nanotubes from the point of view of the quantum graphs. Since there exist chemical double bonds between carbon atoms on a hexagonal lattice with a cylindrical structure corresponding to carbon nanotubes, we study the spectral structure of periodic Schrödinger operators on zigzag nanotubes with multiple bonds of atoms in this paper. Utilizing the Floquet–Bloch theory, the spectrum of the operator consists of the absolutely continuous spectral bands and the flat band. We study the relationship between the number of the chemical bonds and the existence of spectral gaps.

Key Words and Phrases. Carbon nanotube, Zigzag nanotube, Quantum graph, Spectral gap, Band structure, Floquet–Bloch theory, Hill operator.

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1. Introduction and main results

In recent years, we have learned carbons are forming various types of allotropes such as diamond, fullerene, graphene, graphite, carbon nanotube, etc. The electrical conduction for these materials is closely related to the spectral and scattering properties for their corresponding periodic Schrödinger operators. In this paper, we discuss a spectral problem for periodic Schrödinger operators on a generalized model of carbon nanotubes from the point of view of a quantum graph. Here, we denote a generalized model of carbon nanotubes by a nanotube with the multiple chemical bonds between atoms (see Fig. 1).

Let us define periodic Schrödinger operators on zigzag nanotubes with multiple chemical bonds. First, we describe the definition of the corresponding metric graph. We fix \( N \in \mathbb{N} \), which implies the number of hexagons in one layer, and denote the zigzag nanotube with \( N \)-zigzags by \( \Gamma^N \). The precise definition of \( \Gamma^N \) can be defined as follows. For the fixed \( N \), we put \( Z_N = \mathbb{Z} / (N \mathbb{Z}) \) and \( R_N = \sqrt{3} / (4 \sin(\pi/2N)) \). Furthermore, we fix \( N_1, N_2, N_3 \in \mathbb{N} \), which imply the number of chemical bonds of atoms. For each \( j \in \mathcal{J} := \{1, 2, 3\} \), we define \( \mathcal{J}_j = \mathbb{Z} \times Z_N \times \{1, 2, \ldots, N_j\} \). For each \( j \in \mathcal{J} \) and
\((n, k, m_j) \in \mathcal{J}_j\), we define the segment \(\Gamma_{n, j, k, m_j} = \{x = r_{n, j, k, m_j} + t e_{n, j, k, m_j} | 0 \leq t \leq 1\}\), where \(c_k = \cos(\pi k/N)\), \(s_k = \sin(\pi k/N)\), \(\kappa_k = R_N(c_k, s_k, 0)\) and

\[
\begin{align*}
  e_1 &= (0, 0, 1), & e_{n, 1, k, m_1} &= (0, 0, 1), \\
  e_{n, 2, k, m_2} &= \kappa_{n+2k+1} - \kappa_{n+2k} + \frac{e_1}{2}, & e_{n, 3, k, m_3} &= \kappa_{n+2k+2} - \kappa_{n+2k+1} - \frac{e_1}{2}, \\
  r_{n, 1, k, m_1} &= \kappa_{n+2k} + \frac{3n}{2} e_1, & r_{n, 2, k, m_2} &= r_{n, 1, k} + e_1, & r_{n, 3, k, m_3} &= r_{n+1, 1, k}.
\end{align*}
\]

The definition of \(\Gamma_{n, j, k, m_j}\) does not depend on \(m_j\). So, we have \(\Gamma_{n, j, k, 1} = \Gamma_{n, j, k, 2} = \cdots = \Gamma_{n, j, k, N_j}\) for \(j = 1, 2, 3\), but we distinguish \(\Gamma_{n, j, k, \ell}\) and \(\Gamma_{n, j, k, m}\) for distinct \(\ell, m \in \{1, 2, \ldots, N_j\}\). To help our comprehension for the definition of the segment \(\Gamma_{n, j, k, m_j}\), let us see Fig. 2, in which we cut and open \(\Gamma^6\). Putting \(\Gamma^N = \bigcup_{j=1}^3 \bigcup_{(n, k, m_j) \in \mathcal{J}_j} \Gamma_{n, j, k, m_j}\), we obtain the cylindrical metric graph corresponding to the zigzag nanotube with \(N\)-zigzags and \(N_1, N_2, N_3\) chemical bonds. The left and right hand side of Fig. 1 implies \(\Gamma^8\) in the case of \((N_1, N_2, N_3) = (1, 1, 1)\) and \((N_1, N_2, N_3) = (1, 2, 3)\), respectively. In [9, 11], the case of \((N_1, N_2, N_3) = (1, 1, 1)\) has been studied as carbon nanotubes. Now, let us recall that the atomic number of carbon is 6. If we identify the edges of a metric graph as the chemical bonds between carbon atoms, the number of edges around a vertex of carbon nanotubes ought to be 4. Since this implies that there exists the double chemical bonds somewhere in the case of standard carbon nanotubes, we need the model such as \((N_1, N_2, N_3) = (1, 1, 2), (1, 2, 1),\)
These segments are given the orientation from bottom to top. On the line from bottom left to the index of graphene. On the vertical line (heavy line), there exist multiple bonds. We are generally considering the case where there exist plural edges inside this graphene. Cutting and opening the zigzag nanotube $G^6$, we obtain the graphene possessing the multiple bonds. On the line from bottom left to top right, there exist $N_2$ segments $G_{n,2,k,1}, G_{n,2,k,2}, \ldots, G_{n,2,k,N_2}$. Finally, there exist $N_3$ segments $G_{n,3,k,1}, G_{n,3,k,2}, \ldots, G_{n,3,k,N_3}$ on the line from top left to bottom right. The tetrad $n, j, k, m$ implies the index of $G_{n,j,k,m}$.

$(2,1,1)$. Furthermore, we have chances to see various types of nanotubes such as gold nanotubes and boron nanotubes. In considering the model of zigzag nanotubes consisting of atoms except carbons, we are wondering how to describe the difference of the models. Our model establishes a simple generalization at this point. For example, the case $(N_1, N_2, N_3) = (2,2,2)$ corresponds to a fluorine nanotube.

We next define a periodic Schrödinger operator acting on the Hilbert space

$$L^2(G^N) = \bigoplus_{j=1}^{3} \bigoplus_{(n,k,m) \in J_j} L^2(G_{n,j,k,m})$$

equipped with the inner product

$$\langle \psi, \phi \rangle_{L^2(G^N)} = \sum_{j=1}^{3} \sum_{(n,k,m) \in J_j} \langle \psi_{n,j,k,m}, \phi_{n,j,k,m} \rangle_{L^2(G_{n,j,k,m})}$$

for $\psi = (\psi_{n,j,k,m})_{j \in J, (n,k,m) \in J_j}$, $\phi = (\phi_{n,j,k,m})_{j \in J, (n,k,m) \in J_j} \in L^2(G^N)$, where we identify each edge $G_{n,j,k,m}$ as the interval $[0,1]$ and give the local coordinate $x \in [0,1]$ to them because the length of each $G_{n,j,k,m}$ is equal to 1. For $j = 1, 2, 3$ and $(n,k,m) \in J_j$, we abbreviate $y_{n,j,k,m} = y|_{G_{n,j,k,m}}$ for a function $y$ defined on $G^N$ and denote $f'_{n,j,k,m}(1-0)$ and $f'_{n,j,k,m}(+0)$ by $f''_{n,j,k,m}(1)$ and $f''_{n,j,k,m}(0)$. Furthermore, we put $I_{n,j,k,m} = \{ x = r_{n,j,k,m} + t e_{n,j,k,m} | 0 < t < 1 \}$, which can be identified with the open interval $(0,1)$. Picking a real-valued potential $q \in L^2(0,1)$, we define a periodic Schrödinger operator

$$(H_{n,j,k,m})(x) = -f''_{n,j,k,m}(x) + q(x)f_{n,j,k,m}(x)$$
for $x \in (0, 1) \simeq \Gamma^o_{n,j,k,m_j}$, $j = 1, 2, 3$ and $(n, k, m_j) \in J$. Imposing the Kirchhoff condition (which is also called the free boundary condition or the Neumann vertex condition), we obtain a self-adjoint operator $H$ in $L^2(\Gamma^N)$ (see [10]). The Kirchhoff condition consists of the continuity of wave function and no flux condition. For each $n \in \mathbb{Z}$ and $k \in \mathbb{Z}_N$, we take point $A_{n,k}$ and $B_{n,k}$ at the position of Fig. 3. At each $A_{n,k}$, $f \in \text{Dom}(H)$ satisfies

$$-\sum_{m_1=1}^{N_1} f'_{n,1,k,m_1}(1) + \sum_{m_2=1}^{N_2} f'_{n,2,k,m_2}(0) - \sum_{m_3=1}^{N_3} f'_{n,3,k-1,m_3}(1) = 0,$$

$$f_{n,1,k}(1) = \cdots = f_{n,1,k,N_1}(1) = f_{n,2,k,1}(0) = \cdots = f_{n,2,k,N_2}(0) = f_{n,3,k-1,1,N_1}(1).$$

At each $B_{n,k}$, $f \in \text{Dom}(H)$ satisfies

$$-\sum_{m_1=1}^{N_1} f'_{n,1,k,m_1}(1) + \sum_{m_2=1}^{N_2} f'_{n,2,k,m_2}(0) + \sum_{m_1=1}^{N_1} f'_{n,3,k+1,m_1}(0) = 0,$$

$$f_{n,2,k,1}(1) = \cdots = f_{n,2,k,N_2}(1) = f_{n,3,k,1}(0) = \cdots = f_{n,3,k,N_3}(0) = f_{n+1,1,k,0,N_1}(0).$$

The aim of this paper is to investigate the spectrum of $H$, designated by $\sigma(H)$.

To this end, we utilize the same method established in [9, Theorem 1.1]. In the case of $N = 1$ and $(N_1, N_2, N_3) = (1, 2, 3)$, we see that $\Gamma^1$ can be the graph in Fig. 4. The graph $\Gamma^1$ is called the degenerate zigzag nanotube. Let us $N$ operators acting in $L^2(\Gamma^1)$ to attain the unitarily equivalence between the operator $H$ and the direct sum of the $N$ operators. We put $s = e^{2\pi i/\sqrt{N}}$. For $k = 1, 2, \ldots, N$, we define $H_k$ in $L^2(\Gamma^1)$ as follows:

$$(H_k f_{n,j,0,m_j})(x) = -f''_{n,j,0,m_j}(x) + q(x)f_{n,j,0,m_j}(x)$$
for $x \in (0, 1) \simeq \Gamma_{n,j,0,n_j}$, $n \in \mathbb{Z}$, $j \in \mathcal{J}$, and $m_j \in \{1, 2, \ldots, N_j\}$. At $B_n$ in Fig. 4, we impose the Kirchhoff vertex condition: $f \in \text{Dom}(H_k)$ satisfies

$$- \sum_{m_2=1}^{N_2} f'_{n,2,0,m_2}(1) + \sum_{m_3=1}^{N_3} f'_{n,3,0,m_3}(0) + \sum_{m_1=1}^{N_1} f'_{n+1,1,0,m_1}(0) = 0,$$

$$f_{n,2,0,1}(1) = \cdots = f_{n,2,0,N_2}(1) = f_{n,3,0,1}(0) = \cdots = f_{n,3,0,N_3}(0)$$

$$= f_{n+1,1,0,1}(0) = \cdots = f_{n+1,1,0,N_1}(0).$$

At $A_n$ in Fig. 4, we impose the vertex condition

$$- \sum_{m_1=1}^{N_1} f'_{n,1,0,m_1}(1) + \sum_{m_2=1}^{N_2} f'_{n,2,0,m_2}(0) - s^k \sum_{m_3=1}^{N_3} f'_{n,3,0,m_3}(1) = 0,$$

$$f_{n,1,0,m_1}(1) = \cdots = f_{n,1,0,N_1}(1) = f_{n,2,0,1}(0) = \cdots = f_{n,2,0,N_2}(0)$$

$$= s^k f_{n,3,0,1}(1) = \cdots = s^k f_{n,3,0,N_3}(1)$$

for $f \in \text{Dom}(H_k)$. Then, we obtain the unitarily equivalence between $H$ and $\bigoplus_{k=1}^{N} H_k$, and hence we obtain

$$\sigma(H) = \bigcup_{k=1}^{N} \sigma(H_k).$$

Since our spectral problem is reduced to the one-dimensional problem to $H_k$ in this sense, we hereafter examine $\sigma(H_k)$.

In order to describe our theorems, we give notations on the classical theory [1, 12, 18] for the Hill operator $L := -d^2/dx^2 + q$, where $q$ is the same one as the potential of $H$ and is extended to the 1-periodic function on $\mathbb{R}$. Let $\theta(x, \lambda)$ and $\varphi(x, \lambda)$ be the linearly independent solutions to the Schrödinger equation

$$-y''(x, \lambda) + q(x)y(x, \lambda) = \lambda y(x, \lambda), \quad x \in \mathbb{R}, \ \lambda \in \mathbb{C}$$

Fig. 4. The degenerate zigzag nanotube $I^1$. On the Spectra of Schrödinger Operators 259
as well as the initial conditions \( \theta(0, \lambda) = 1, \theta'(0, \lambda) = 0 \) and \( \varphi(0, \lambda) = 0, \varphi'(0, \lambda) = 1 \), respectively. Then, we introduce

\[
A_-(\lambda) = \frac{\theta(1, \lambda) - \varphi'(1, \lambda)}{2}
\]

and the spectral discriminant

\[
A(\lambda) := \frac{\theta(1, \lambda) + \varphi'(1, \lambda)}{2},
\]

which are entire in \( \lambda \in \mathbb{C} \) because \( \theta(x, \lambda), \varphi(x, \lambda), \varphi'(x, \lambda) \) are entire in \( \lambda \in \mathbb{C} \). The spectrum of \( L \) can be characterized by \( A(\lambda) \) as

\[
\sigma(L) = \sigma_{ac}(L) = \{ \lambda \in \mathbb{R} \mid |A(\lambda)| \leq 1 \} = \bigcup_{j \in \mathbb{N}} [\lambda_{2j-2}, \lambda_{2j-1}],
\]

where \( \lambda_0, \lambda_1, \lambda_2, \ldots \) are zeroes of \( A(\lambda) \pm 1 \) and are labeled in increasing order. The zeroes satisfy the inequality \( \lambda_0 < \lambda_1 < \lambda_2 < \lambda_3 < \lambda_4 < \cdots \). For \( j \in \mathbb{N} \), the interval \([\lambda_{2j-2}, \lambda_{2j-1}]\) is called the \( j \)th band of \( \sigma(L) \), counted from the bottom. Two consecutive bands \([\lambda_{2j-2}, \lambda_{2j-1}]\) and \([\lambda_{2j}, \lambda_{2j+1}]\) are separated by \((\lambda_{2j-1}, \lambda_{2j})\), which is referred as the \( j \)th spectral gap of \( L \). Let \( \sigma_D(L) \) be the Dirichlet spectrum, namely, the spectrum of the eigenvalue problem \(-y'' + qy = \lambda y\) with \( y(0) = y(1) = 0 \). Since \( \sigma_D(L) \) is discrete, we denote the \( k \)th Dirichlet eigenvalues by \( \mu_k \). Then, we have \( \sigma_D(L) = \{ \lambda \in \mathbb{R} \mid \varphi(1, \lambda) = 0 \} \) and \( \mu_n \in [\lambda_{2n-1}, \lambda_{2n}] \) for each \( n \in \mathbb{N} \). Let \( \{\eta_j\}_{j=0}^\infty \) be the zeroes of \( A(\lambda) \), which are arranged in increasing order. Then, we have \( \eta_1 < \mu_1 < \eta_2 < \mu_2 < \cdots \). This inequality is important to state Theorem 1.8.

Under these preparations, we construct a spectral discriminant for \( H_k \).

For convenience, we put \( H_0 = H_N \). For \( k = 0, 1, 2, \ldots, N \), we note that \( \cos^2(\pi k/N) = (N_2 - N_3)^2/(2(N_2^2 + N_3^2)) \) is equivalent to

\[
\left( N_2 + N_3 \cos \frac{2\pi k}{N} \right)^2 + N_3^2 \sin^2 \frac{2\pi k}{N} = 0.
\]

We prepare the set

\[
K_0 = \left\{ k = 0, 1, 2, \ldots, N \mid \cos^2 \frac{\pi k}{N} = \frac{(N_2 - N_3)^2}{2(N_2^2 + N_3^2)} \right\}. \]

For \( k = 0, 1, 2, \ldots, N \) and \( \lambda \in \mathbb{C} \), we define

\[
D(k, \lambda) = \begin{cases} \frac{F(k, \lambda)}{2N_1 \sqrt{(N_2 + N_3 \cos \frac{2\pi k}{N})^2 + N_3^2 \sin^2 \frac{2\pi k}{N}}} & \text{if } k \notin K_0, \\ F(k, \lambda) & \text{otherwise}, \end{cases}
\]
where
\[ F(k, \lambda) = (N_1 + N_2 + N_3)^2 \mathcal{A}^2(\lambda) - (N_1 - N_2 + N_3)^2 \mathcal{A}^2(\lambda) - \{N_1^2 + (N_2 - N_3)^2\} - 4N_2N_3 \cos^2 \frac{\pi k}{N}. \]

Furthermore, we denote the flat band of \( H_k \) by \( \sigma_\infty(H_k) \) for \( k = 0, 1, 2, \ldots, N \). We recall that \( \sigma_\infty(H_k) \) implies the set of all eigenvalues of \( H_k \) with infinite multiplicities. We use the standard notation \( \sigma_{ac}(H_k) \) for the absolutely continuous spectrum of \( H_k \). Then, we first obtain the following:

**Theorem 1.1.** For \( k = 0, 1, 2, \ldots, N \), we have \( \sigma(H_k) = \sigma_\infty(H_k) \cup \sigma_{ac}(H_k) \).

(a) If \( k \in K_0 \), then we have
\[ \sigma_\infty(H_k) = \sigma_D(L) \cup \{ \lambda \in \mathbb{R} \mid F(k, \lambda) = 0 \} \quad \text{and} \quad \sigma_{ac}(H_k) = \emptyset. \]

(b) If \( k \notin K_0 \), then we have
\[ \sigma_\infty(H_k) = \sigma_D(L) \quad \text{and} \quad \sigma_{ac}(H_k) = \{ \lambda \in \mathbb{R} \mid D(k, \lambda) \in [-1, 1] \}. \]

Furthermore, we have \( \sigma_{ac}(H_k) = \sigma_{ac}(H_{N-k}) \) for \( k = 0, 1, 2, \ldots, N \).

**Remark 1.2.** In the case where \( N_2 = N_3 \) and \( N \) is odd, we have \( k \notin K_0 \) for all \( k = 0, 1, 2, \ldots, N \) because of \( \cos^2(\pi k/N) \neq 0 \). Thus, the case is not included in Theorem 1.1 (a). In this sense, Theorem 1.1 (a) is a generalization of [9, Theorem 1.3 (iii)]. In the case of \( N_1 = N_2 = N_3 = 1 \) and \( N = 2l \), then \( \ell \in K_0 \). Thus, there exists eigenvalues except for the Dirichlet eigenvalues. So, Theorem 1.1 (b) is a generalization of [11, Theorem 4.3 (vii)].

For \( c \in [-1, 1] \) and \( k = 0, 1, 2, \ldots, N \), we put

\[ A_\pm(c, k) = \pm \frac{1}{N_1 + N_2 + N_3} \sqrt{\alpha(N_1, N_2, N_3, c, k)}, \]

where
\[ \alpha(N_1, N_2, N_3, c, k) = N_1^2 + (N_2 - N_3)^2 + 4N_2N_3 \cos^2 \frac{\pi k}{N} + 2N_1c \sqrt{(N_2 - N_3)^2 + 4N_2N_3 \cos^2 \frac{\pi k}{N}}. \]

Then, we first obtain the following results for \( \sigma_{ac}(H_k) \) in the unperturbed case.

**Theorem 1.3.** Assume that \( k \notin K_0 \) and \( q \equiv 0 \). Then, we obtain \( \sigma_{ac}(H_k) = \bigcup_{n=1}^{\infty} B_n(k) \), where
for \( j \in \mathbb{N} \). Namely, the absolutely continuous spectrum has the band-gap structure. The interval \( B_n(k) \) implies the \( n \)th spectral gap for \( H_k \). For \( j \in \mathbb{N} \), \( B_j(k) \) and \( B_{j+1}(k) \) is separated the spectral gap \( G_j(k) \) defined as

\[
G_{j-3}(k) = \{(2(j - 1)\pi + \arccos A_+(1,k))^2, 2(j - 1)\pi + \arccos A_+(-1,k)\}^2, \\
G_{j-2}(k) = \{(2(j - 1)\pi + \arccos A_+(1,k))^2, (2j\pi - \arccos A_-(1,k))^2\}, \\
G_{j-1}(k) = \{(2j\pi - \arccos A_-(1,k))^2, 2(j - 1)\pi + \arccos A_-(-1,k)\}^2, \\
G_j(k) = \{(2j\pi - \arccos A_+(1,k))^2, (2j\pi + \arccos A_+(1,k))^2\}.
\]

**Remark 1.4.** Assume that \( k \notin K_0 \) and \( q \equiv 0 \). Then, for \( j \in \mathbb{N} \), we have

\[
B_{j-3}(k) \subset \left[ 4(j - 1)^2\pi^2, \left( 2(j - 1)\pi + \frac{\pi}{2} \right)^2 \right], \\
B_{j-2}(k) \subset \left[ \left( 2(j - 1)\pi + \frac{\pi}{2} \right)^2, \left( 2(j - 1)\pi + \pi \right)^2 \right], \\
B_{j-1}(k) \subset \left[ (2j\pi - \pi)^2, \left( 2j\pi - \frac{\pi}{2} \right)^2 \right], \\
B_{j}(k) \subset \left[ \left( 2j\pi - \frac{\pi}{2} \right)^2, (2j\pi)^2 \right].
\]

Next, we describe results for \( \sigma_{\text{ac}}(H) \) in the unperturbed case. To this aim, we define the set

\[
K = \left\{ k \notin K_0 \mid \cos^2 \frac{\pi k}{N} = \frac{N_1^2 - (N_2 - N_3)^2}{4N_2N_3} \right\}.
\]

Furthermore, we put \( \rho = \min_{k \notin K_0} |\cos^2(\pi k/N) - (N_1^2 - (N_2 - N_3)^2)/(4N_2N_3)| \) and

\[
k^* = \min \left\{ k \notin K_0 \mid \left| \cos^2 \frac{\pi k}{N} - \frac{N_1^2 - (N_2 - N_3)^2}{4N_2N_3} \right| = \rho \right\}.
\]
If \( K \neq \emptyset \), we see that \( k^* \in K \) and \( k^* \) is uniquely determined. For \( j \in \mathbb{N} \), we define
\[
B_j = \bigcup_{k \neq K_0} B_j(k).
\]

**Theorem 1.5.** Assume that \( q \equiv 0 \).

(i) If \( K \neq \emptyset \), then we have \( B_j = \{(\pi(j-1)/2)^2, (\pi j/2)^2\} \) for \( j \in \mathbb{N} \), and hence \( \sigma_{ac}(H) = \bigcup_{j=1}^\infty B_j = [0, \infty) \). Namely, every spectral gap is degenerate.

(ii) Assume that \( K = \emptyset \). Then, we obtain \( \sigma_{ac}(H) = \bigcup_{j=1}^\infty B_j \), where
\[
B_{4j-3} = [4(j-1)^2 \pi^2, \{2(j-1)\pi + \arccos A_+(1, k^*)\}^2],
B_{4j-2} = [(2(j-1)\pi + \arccos A_+(-1, k^*))^2, (2j-1)^2 \pi^2],
B_{4j-1} = [(2j-1)^2 \pi^2, \{2(j-1)\pi + (2\pi - \arccos A_-(-1, k^*))\}^2],
B_{4j} = [(2j\pi - \arccos A_+(-1, k^*))^2, 4j^2 \pi^2]
\]
for \( j \in \mathbb{N} \). The spectral gap \( G_j \) between \( B_j \) and \( B_{j+1} \) satisfies \( G_{2j} = \emptyset \),
\[
G_{4j-3} = \{(\pi(j-1)\pi + \arccos A_+(-1, k^*))^2, \{(2(j-1)\pi + \arccos A_-(-1, k^*))^2\} \neq \emptyset,
G_{4j-1} = \{(2j\pi - \arccos A_-(-1, k^*))^2, \{2j\pi - \arccos A_+(-1, k^*)\}^2\} \neq \emptyset
\]
for \( j \in \mathbb{N} \).

**Example 1.6.** Let \( N = 3, N_1 = 4, N_2 = 6, N_3 = 4 \). Then, \( |\cos^2(\pi k/3) - 1/8| \) takes its minimum \( \rho = 1/8 \) for \( k = 1, 2 \). So, we have \( K = \emptyset \) and \( k^* = 1 \). Thus, we obtain \( A_+(-1, k^*) = \sqrt{11 - 4\sqrt{7}/7} = (\sqrt{7} - 2)/7 \) and \( A_-(-1, k^*) = -\sqrt{11 - 4\sqrt{7}/7} = (2 - \sqrt{7})/7 \). Theorem 1.3 yields \( B_1 = [0, (\arccos((\sqrt{7} - 2)/7))^2], B_2 = [(\arccos((2 - \sqrt{7})/7))^2, \pi^2], B_3 = [\pi^2, (2\pi - \arccos((2 - \sqrt{7})/7))^2], B_4 = [(2\pi - \arccos((\sqrt{7} - 2)/7))^2, 4\pi^2] \) and so on.

We take further examples. In the case where \( q \equiv 0 \), we can adequately find the difference between single edge and multiple edges. Let \( N_{k_0} = (N_2 - N_3)^2/(2(N_2^2 + N_3^2)) \) and \( N_K = (N_1^2 - (N_2 - N_3)^2)/(4N_2N_3) \).

**Example 1.7.** Assume that \( q \equiv 0 \). Since it follows by Theorem 1.5 that \( G_{2j} = \emptyset \), the existence of non-degenerate spectral gaps depends on only the odd-indexed spectral gaps \( G_{2j-1} \). We have the following examples.

(1) Let \( (N_1, N_2, N_3) = (1, 1, p) \), where \( p \in \mathbb{N} \). Then, we have \( N_{k_0} = (1 - p)^2/(2(1 + p^2)) \) and \( N_K = p(2 - p)/4 \). Thus, we obtain the followings:
(a) Assume that \( p \geq 3 \). Then, we have \( K = \emptyset \). This together with Theorem 1.5 (ii) yields \( G_{2j-1} \neq \emptyset \) for all \( j \in \mathbb{N} \).

(b) Assume that \( p = 2 \). Then, we have \( N_{K_0} = 1/10 \) and \( N_K = 0 \). So, we have \( K \neq \emptyset \) if and only if \( k = N/2 \in \mathbb{N} \). Thus, we obtain the followings:
- If \( N/2 \in \mathbb{N} \), then \( G_{2j-1} = \emptyset \) for all \( j \in \mathbb{N} \).
- If \( N/2 \notin \mathbb{N} \), then \( G_{2j-1} \neq \emptyset \) for all \( j \in \mathbb{N} \).

(c) Assume that \( p = 1 \), whose case has been already discussed in [9, Theorem 1.4] and [11, Theorem 4.3 (viii)]. Then, we have \( N_{K_0} = 0 \) and \( N_K = 1/4 \). So, we have \( K \neq \emptyset \) if and only if \( k = N/3, 2N/3 \in \mathbb{N} \). Thus, we obtain the followings:
- If \( N/3 \in \mathbb{Z} \), then \( G_{2j-1} = \emptyset \) for all \( j \in \mathbb{N} \).
- If \( N/3 \notin \mathbb{Z} \), then \( G_{2j-1} \neq \emptyset \) for all \( j \in \mathbb{N} \).

Furthermore, we have \( K_0 = \emptyset \) if and only if \( N/2 \in \mathbb{N} \). Thus, we obtain the followings:
- If \( N \) is odd, then \( \sigma_0(\mathcal{H}) = \sigma_D(\mathcal{L}) \) ([9, Theorem 1.4]).
- If \( N \) is even, then \( \sigma_0(\mathcal{H}) = \sigma_D(\mathcal{L}) \cup \{ \lambda \in \mathbb{R} \mid F(N/2, \lambda) = 0 \} \) ([11, Theorem 4.3 (viii)]).

(2) Let \((N_1, N_2, N_3) = (p, 1, 1)\), where \( p = 2, 3, \ldots \). Then, we have \( N_{K_0} = 0 \) and \( N_K = p^2/4 \). Thus, we see that \( K_0 = \emptyset \) if and only if \( k = N/2 \in \mathbb{N} \). Furthermore, we have the followings:
- If \( p \geq 3 \), then we have \( K = \emptyset \) and hence \( G_{2j-1} \neq \emptyset \).
- If \( p = 2 \), then we have \( K = \{0, N\} \neq \emptyset \) and hence \( G_{2j-1} = \emptyset \).

(3) Let \((N_1, N_2, N_3) = (p, p, p)\), where \( p \in \mathbb{N} \). Then, we have \( N_{K_0} = 0 \) and \( N_K = 1/4 \). Thus, we obtain
\[
K_0 = \begin{cases} 
\{ \frac{N}{3} \} \quad \text{if } \frac{N}{3} \in \mathbb{N}, \\
\emptyset \quad \text{if } \frac{N}{3} \notin \mathbb{N}
\end{cases} \\
K = \begin{cases} 
\{ \frac{N}{3}, \frac{2N}{3} \} \quad \text{if } \frac{N}{3} \in \mathbb{N}, \\
\emptyset \quad \text{if } \frac{N}{3} \notin \mathbb{N}
\end{cases}
\]

This result does not depend on \( p \). Furthermore, we obtain the followings:
- If \( N/3 \in \mathbb{N} \), then we have \( G_{2j-1} \neq \emptyset \) for all \( j \in \mathbb{N} \).
- If \( N/3 \notin \mathbb{N} \), then we have \( G_{2j-1} = \emptyset \) for all \( j \in \mathbb{N} \).

The cases of \( p = 1 \) and \( p = 2 \) correspond to boron nanotubes and fluorine nanotubes, respectively.

(4) Let \((N_1, N_2, N_3) = (7, 5, 3)\). Then, it follows by \( N_{K_0} = 1/17 \) and \( N_K = 3/4 \) that \( K_0 \cap K = \emptyset \). Moreover, we have \( K \neq \emptyset \) if and only if \( k = N/6, 5N/6 \in \mathbb{N} \). Thus, we obtain the followings:
- If \( N/6 \notin \mathbb{N} \), then we have \( G_{2j-1} = \emptyset \) for all \( j \in \mathbb{N} \).
- If \( N/6 \in \mathbb{N} \), then we have \( G_{2j-1} \neq \emptyset \) for all \( j \in \mathbb{N} \).

Especially, we obtained the case where \( N/3 \in \mathbb{N} \) but \( G_{2j-1} = \emptyset \) for all \( j \in \mathbb{N} \), which happen if \( N = 3, 9, 15, \ldots \). This does not happen in the case of \((N_1, N_2, N_3) = (1, 1, 1)\).
Let \((N_1, N_2, N_3) = (4, 1, 2)\) and \(N = 6\). Then, we have \(N_{K_0} = 1/10\) and \(N_K = 15/8\). For \(k = 0, 1, 2, \ldots, 6\), we have \(\cos^2(\pi k/6) \neq N_K, N_{K_0}\). Thus, we derive \(K_0 = \emptyset\) and \(K = \emptyset\). It follows by Theorem 1.4 that \(\sigma_\infty(H) = \sigma_d(L)\). It follows by [11, Theorem 4.3 (vii)] that \(\sigma_\infty(H) \supseteq \sigma_d(L)\) if \(N_1 = N_2 = N_3 = 1\) and \(N\) is even.

Let \((N_1, N_2, N_3) = (5, 4, 3)\). Then, we have \(N_{K_0} = 1/50\) and \(N_K = 1/2\). Thus, we see that \(\cos^2(\pi k/N) = 1/2\) is equivalent to \(k = N/4, 3N/4 \in N\).

This yields the followings:

- If \(N/4 \in \mathbb{Z}\), then we have \(G_{2j-1} = \emptyset\) for all \(j \in N\).
- If \(N/4 \notin \mathbb{Z}\), then we have \(G_{2j-1} \neq \emptyset\) for all \(j \in N\).

Next, we deal with the perturbed case.

**Theorem 1.8.** Let \(k \notin K_0\). Then, there exists real sequence

\[
\lambda_{k,0}^+ < \lambda_{k,1}^- \leq \lambda_{k,1}^+ < \lambda_{k,2}^- \leq \cdots < \lambda_{k,n}^- \leq \lambda_{k,n}^+ < \cdots
\]

such that \(\sigma_{ac}(H_k) = \bigcup_{j=1}^\infty [\lambda_{k,j-1}^+, \lambda_{k,j}^-]\). Furthermore, we have the followings:

(A) If \(k \neq 0, N\), then we have \(\lambda_{k,2j} \neq \lambda_{k,2j}'\).

(B) If \(K = \emptyset\), then we have \(\lambda_{k,2j-1} \neq \lambda_{k,2j-1}'\) for all \(k = 0, 1, \ldots, N\).

(C) If \(K \neq \emptyset\), then we have \(\lambda_{k,2j-1} \neq \lambda_{k,2j-1}'\) for all \(k \neq k^*, N - k^*\).

(D) For each \(j \in N\), we have \(\lambda_{k,2j-1} \leq \eta_j \leq \lambda_{k,2j} < \lambda_{k,2j}' \leq \mu_j \leq \lambda_{k,2j}'\).

Due to the inequalities of Theorem 1.8 (D), we can construct the band-gap structure of \(\sigma_{ac}(H)\) as follows. Let us define \(\lambda_0^+ = \min_{k \notin K_0} \lambda_{k,0}^+\), \(\lambda_j^- = \max_{k \notin K_0} \lambda_{k,j}^-\), and \(\lambda_j^+ = \min_{k \notin K_0} \lambda_{k,j}^+\) for all \(j \in N\). Since \(\sigma_{ac}(H) = \bigcup_{k \notin K_0} \sigma_{ac}(H_k)\), we have an expression

\[
\sigma_{ac}(H) = \bigcup_{j=1}^\infty [\lambda_{j-1}^+, \lambda_j^-],
\]

which implies the band-gap structure of \(\sigma_{ac}(H)\). For each \(j \in N\), we refer to \(B_j := [\lambda_{j-1}^+, \lambda_j^-]\) and \(G_j := (\lambda_j^-, \lambda_j^+)\) as the \(j\)th band and gap of \(\sigma(H)\), respectively. Two consecutive bands have a possibility to merge. Due to Theorem 1.8 (B), we immediately obtain the following statement:

**Theorem 1.9.** If \(K = \emptyset\), then we have \(G_{2j-1} \neq \emptyset\) for all \(j \in N\).

- Assume that \(K \neq \emptyset\). For \(j \in N\), we have \(\lambda_{k^*,2j-1} = \lambda_{k^*,2j-1}'\) if and only if \(G_{2j-1} = \emptyset\).

- For \(j \in N\), we have \(\lambda_{0,2j}^- = \lambda_{0,2j}^+\) if and only if \(G_{2j} = \emptyset\).

Let us give a qualitative estimate for an existence of a spectral gap of \(\sigma(H)\).
Theorem 1.10. Assume that $q$ is a gap-opening even potential for the operator $L$. Namely, we assume that $q(x) = q(1-x)$ holds true for $x \in (0, 1)$ and $\sigma(L)$ has a spectral gap. Then, we have $\sigma(H)$ has a spectral gap for any combination of $N_1, N_2, N_3$.

Spectra of quantum graphs have a close relationship to a discrete Schrödinger operator. The relationship has been developed in [2, 14, 15] with the theory of the so-called boundary triplet. From the view point of his results, we see that the number of edges $(N_1, N_2, N_3)$ can be embedded as the potential of a corresponding tight binding model. Let us recall his results from [14] (see also [15]) in order to ensure a mutual understanding of our quantum graph and a discrete Schrödinger operator on $\Gamma$. Let $E$ and $V$ be the set of edges and vertexes of our zigzag nanotube $\Gamma$. For each $e \in E$, we define $i(e)$ and $\tau(e)$ as the initial and terminal vertex of $e$. For each $v \in V$, the number of outgoing edges and incoming edges are denoted by $\text{outdeg}_i(v)$ and $\text{indeg}_i(v)$, respectively. Namely, we have $\text{indeg}(A_{n,j}) = N_1 + N_3$, $\text{outdeg}(A_{n,j}) = N_2$, $\text{indeg}(B_{n,j}) = N_2$ and $\text{outdeg}(B_{n,j}) = N_1 + N_3$ for $n \in \mathbb{Z}$ and $j = 1, 2, 3$ (see Fig. 3). Let $\text{deg}(v)$ be the degree of $v \in V$. Then, we have $\text{deg}(v) = N_1 + N_2 + N_3$ for each $v \in V$. Furthermore, we put $E^v = \{e \in E\mid i(e) = v\}$ and $E^v = \{e \in E\mid \tau(e) = v\}$ for each $v \in V$. We consider the Hilbert space $l^2(\Gamma)$ equipped with the weighted scalar product $(f, g)_{\Gamma} = \sum_{v \in V} \text{deg}(v)f(v)\overline{g(v)}$. We define a discrete Laplacian in $l^2(\Gamma)$ as

$$A_{\Gamma}h(v) = \frac{1}{\text{deg}(v)} \left( \sum_{e \in E^v} h(\tau(e)) + \sum_{e \in E^v} h(i(e)) \right),$$

which is a bounded self-adjoint operator in $l^2(\Gamma)$. On the other hand, we define a closed operator $T$ in $L^2(\Gamma)$ as

$$\text{Dom}(T) = \{f \in H^2(\Gamma)\mid f \text{ is continuous at each } v \in V\},$$

$$(Tf_{n,j,k,m})(x) = -f^\prime_{n,j,k,m}(x) + q(x)f_{n,j,k,m}(x)$$

for $x \in (0, 1) \simeq \Gamma_{n,j,k,m}$, $j = 1, 2, 3$ and $(n, k, m) \in \mathcal{J}$. For $f \in H^2(\Gamma)$ and $v \in V$, we define

$$f'(v) = \sum_{e \in E_v} f'(i(e)) - \sum_{e \in E_v} f'(\tau(e))$$

and introduce operators $\pi : H^2(\Gamma) \to l^2(\Gamma)$ and $\pi' : H^2(\Gamma) \to l^2(\Gamma)$ as

$$\pi f = (f(v))_{v \in V} \quad \text{and} \quad \pi' f = \left( \frac{f'(v)}{\text{deg}(v)} \right)_{v \in V}.$$
Then, it is known that \((l^2(\eta^N), \pi, \pi')\) is a boundary triplet of \(T\). Furthermore, we define a bounded operator in \(l^2(\eta^N)\) for \(z \notin \sigma_d(L)\) as
\[
(M(z)h)(v) = \frac{-1}{\varphi(1, z)}(-A_{F^N} + p(v, z))h(v), \quad h \in l^2(\eta^N),
\]
where
\[
p(v, z) = \frac{\text{outdeg}(v)}{\deg(v)} \varphi(1, z) + \frac{\text{indeg}(v)}{\deg(v)} \varphi'(1, z).
\]
Note that \(M(z)\) is called the Weyl function for \(T\). Utilizing Krein's resolvent formula, we have
\[
\sigma(H) = \sigma_d(L) \cup \Sigma,
\]
where
\[
\Sigma = \{ z \in R \setminus \sigma_d(L) \mid 0 \in \sigma(M(z)) \}.
\]
Recall that \(\varphi(1, z) \neq 0\) for \(z \notin \sigma_d(L)\). Thus, we see that \(z \notin \sigma_d(L)\) is in \(\sigma(H)\) if and only if a discrete Schrödinger operator \(-A_{F^N} + p(v, z)\) has 0 as a spectrum. In this sense, the number of edges of \(H\) appears as the potential \(p(v, z)\) of the corresponding discrete Schrödinger operator. Consider the spectral problem corresponding to \(-A_{F^N} + p(x, z)\):
\[
-A_{F^N}h(v) + p(z, v)h(v) = 0.
\]
Under a special assumption \(q\) is even or \(\text{indeg}(v) = \text{outdeg}(v)\), i.e., \(N_1 + N_3 = N_2\), the relationship between \(\sigma(H)\) and \(\sigma(A_{F^N})\) is more simplified. Actually, if \(q\) is even or \(\text{indeg}(v) = \text{outdeg}(v)\), then the potential is given by the Hill's discriminant: \(p(v, z) = \Delta(z)\). Therefore, we obtain \(\Sigma = \Delta^{-1}(\sigma(A_{F^N})) \setminus \sigma_d(L)\). Note that the Hill's discriminant \(\Delta\) is a homeomorphism between each band of \(\sigma(L)\) and \([-1, 1]\). Thus, we have the followings:

- ([14]) If there exists a spectral gap for the discrete Schrödinger operator \(A_{F^N}\) for some combination of \((N_1, N_2, N_3)\), the spectrum of \(H\) also has a spectral gap for any potential \(q\) satisfying the assumption: \(q\) is even or \(\text{indeg}(v) = \text{outdeg}(v)\).

We stress that Pankrashkin developed in [2, 14] the relationship between a quantum graph and a tight binding model inside a magnetic field.

As stated here, our results relates to the existence of spectral gap of the corresponding tight binding model. In this paper, we directly examine the spectra of our Hamiltonians utilizing the Floquet–Bloch theory. Nowadays, we can find numerous results of spectra of periodic quantum graphs. Let us pick up some of those fruitful properties. Originally, a notion of quantum graphs appeared in the 1930s in order to examine free electrons in organic molecules [16]. In the 1990s, the spectral theory of quantum graphs has got actively discussed after the work [6]. P. Exner dealt with spectral properties of free Schrödinger operators with \(\delta\) and other class of point interactions on a
rectangular lattice. Making use of the Floquet–Bloch theory for his quantum graph, he proved the existence of the band structure of its spectrum, whose properties depends on number-theoretic properties of the sizes of rectangular. The Floquet–Bloch theory yields numerous spectral results for periodic quantum graphs. Spectral results for periodic Schrödinger operators on carbon nanostructures has been studied in the representative papers [9, 11]. In [11], spectra of periodic Schrödinger operators on graphene and all class of carbon nanotubes have been discussed. The structure of carbon nanotubes can be obtained by taking the quotient of the hexagonal lattice with respect to some equivalence relation. As a result of the quotient, carbon nanotubes are classified into three classes: zigzag, armchair and chiral nanotubes. Kuchment and Post [11] obtained the dispersion relation for graphene. Furthermore, they also derived the dispersion relation to carbon nanotubes by cutting the dispersion relation to graphene form a suitable direction. They found the so-called Dirac point, which plays an important role in the theory of the topological insulator, in the graph of the dispersion relation to the graphene in the case of the free potential. In [9], Korotyaev and Lobanov gave an unitarily equivalence between the quantum graph on their zigzag nanotubes and the direct sum of its corresponding Hamiltonians on a one-dimensional periodic graph with necklace structure called the degenerate zigzag nanotube (see Fig. 4). This equivalence simplified the analysis of periodic Schrödinger operator on zigzag nanotubes. They proved that the spectra of their operators have the band-gap structure consisting of the absolutely continuous spectrum and the set of eigenvalues with infinite multiplicities. The latter set is called the flat band. Korotyaev and Lobanov also gave the asymptotic of spectral band edges, which formulate a further result of the inverse spectral theory. There are further results on the spectra of carbon nanostructures [3, 4, 5, 7, 8]. In [4], Do and Kuchment studied the spectrum of the graphyne, which consists of the hexagons and rhombuses. After this work, Do studied the spectrum of the graphyne with the cylindrical structure in [3]. Exner and Turek [7] studied the relationship between the number of spectral gaps and the ratios of the lengths of edges for free Schrödinger operators on a dilated hexagonal lattice. Korotyaev [8] has studied the effective masses of periodic Schrödinger operators in a uniform magnetic field. In [5], Duclos, Exner and Turek studied the free Schrödinger operator on the metric graph with the necklace structure (like Fig. 2) in the straight and the bending case.

In the next section, we give the proof of theorems.

2. Proof of Theorems

Let us give the proof of theorems stated in §1.
Proof of Theorem 1.1. We first construct infinitely many linearly independent eigenfunctions of $H_k$ for $\lambda \in \sigma(L)$. Let us pick a $\lambda \in \sigma(L)$ arbitrarily and fix it. Put $\eta = 1 - s^k c^2$, where $s = e^{2\pi i / N}$ and $c = \varphi'(1, \lambda)$.

If $\eta = 0$, then we define the function $u^{(0)} = (u^{(0)}_{n,j,0,m_j}(x, \lambda))_{n \in \mathbb{Z}, j \in \mathcal{J}, m_j = 1, \ldots, N_j} \in \text{Dom}(H_k)$ by

$$u^{(0)}_{0,1,0,m_1}(x, \lambda) = 0, \quad u^{(0)}_{0,2,0,m_2}(x, \lambda) = \frac{\varphi(x, \lambda)}{N_2}, \quad u^{(0)}_{0,3,0,m_3}(x, \lambda) = \frac{c \varphi(x, \lambda)}{N_3},$$

and $u^{(0)}_{n,j,0,m_j}(x, \lambda) = 0$ for $n \in \mathbb{Z}\{0\}$, $j \in \mathcal{J}$, $m_j = 1, 2, \ldots, N_j$. If $\eta \neq 0$, then we define the function $u^{(0)} = (u^{(0)}_{n,j,0,m_j}(x, \lambda))_{n \in \mathbb{Z}, j \in \mathcal{J}, m_j = 1, \ldots, N_j} \in \text{Dom}(H_k)$ by

$$u^{(0)}_{0,1,0,m_1}(x, \lambda) = 0, \quad u^{(0)}_{0,2,0,m_2}(x, \lambda) = -\frac{s^k c \varphi(x, \lambda)}{N_2},$$

$$u^{(0)}_{0,3,0,m_3}(x, \lambda) = -\frac{\varphi(x, \lambda)}{N_3}, \quad u^{(0)}_{1,1,0,m_1}(x, \lambda) = \frac{\eta \varphi(x, \lambda)}{N_1},$$

and $u^{(0)}_{n,j,0,m_j}(x, \lambda) = 0$ for $n \in \mathbb{Z}\{0\}$, $j \in \mathcal{J}$, $m_j = 1, 2, \ldots, N_j$. Furthermore, we define $u^{(n)} = (u^{(n)}_{p-n,j,0,m_j}(x, \lambda))_{p \in \mathbb{Z}, j \in \mathcal{J}}$ for each $n \in \mathbb{Z}$. We can directly make sure that $\{u^{(n)}\}_{n \in \mathbb{Z}} \subset \text{Dom}(H_k)$. Note that $u^{(n)}_{n,j,0,m_j}(x, \lambda)$ solves the equation $-u'' + qu = \lambda u$ on the edge $\Gamma_{n,j,0,m_j}$. By the definition of $u^{(n)}$, its support is compact. Since $\text{supp}(u^{(n)}) \neq \text{supp}(u^{(m)})$ for distinct $n, m \in \mathbb{Z}$, we see that $u^{(n)}$ and $u^{(m)}$ are linearly independent for distinct $n, m \in \mathbb{Z}$. Since we obtained infinitely many linearly independent eigenfunctions, we conclude that $\lambda \in \sigma_{\infty}(H_k)$. Namely, we have $\sigma_D(L) \subset \sigma_{\infty}(H_k)$ for each $k = 1, 2, \ldots, N$.

We next examine the set $\sigma(H_k) \setminus \sigma(L)$ by using a direct integral decomposition for $H_k$ for each $k = 1, 2, \ldots, N$ (see [18]). For a quasimomentum $\mu \in [0, 2\pi)$, we define the Hilbert space $\mathcal{H}_{\mu} = \bigoplus_{j=1}^{r} \bigoplus_{m_j=1}^{N_j} L^2(\Gamma_{0,j,0,m_j})$. We consider the unitary operator $U : L^2(\Gamma^1) \to \mathcal{H}$ defined as

$$(Uf)(x, \mu) = \sum_{p \in \mathbb{Z}} e^{ip\mu} f_p(x - p, \mu),$$

$$f = (f_n)_{n \in \mathbb{Z}} = (f_{n,j,0,m_j})_{n \in \mathbb{Z}, j \in \mathcal{J}, m_j = 1, 2, \ldots, N_j} \in L^2(\Gamma^1),$$

where

$$\mathcal{H} = \int_{[0, 2\pi]} \mathcal{H}_{\mu} d\mu = L^2\left([0, 2\pi), \mathcal{H}_{\mu}, \frac{d\mu}{2\pi}\right).$$

Moreover, we define a fiber operator $H_k(\mu)$ in $\mathcal{H}_{\mu}$ defined as

$$(H_k(\mu)f_{j,m_j})(x) = -f''_{j,m_j}(x) + q(x)f_{j,m_j}(x).$$
for \( x \in (0, 1) \simeq I^o_{0,j,0,m_j}, \ j \in \mathcal{J}, \ m_j = 1, 2, \ldots, N_j \). Let a function \( f = (f_j, m_j)_{j \in \mathcal{J}, m_j = 1, 2, \ldots, N_j} \in \text{Dom}(H_k) \) be imposed the boundary condition

\[
(2.1) \quad - \sum_{m_j=1}^{N_1} f'_{1,m_j}(1) + \sum_{m_j=1}^{N_2} f'_{2,m_j}(0) - s^k \sum_{m_j=1}^{N_1} f'_{3,m_j}(1) = 0,
\]

\[
(2.2) \quad f_{1,1} = \cdots = f_{1,N_1}(1) = f_{2,1}(0) = \cdots = f_{2,N_2}(0) = s^k f_{3,1}(1) = \cdots = s^k f_{3,N_3}(1)
\]

at \( A_n \) in Fig. 3, and

\[
(2.3) \quad - \sum_{m_j=1}^{N_2} f'_{2,m_j}(1) + \sum_{m_j=1}^{N_3} f'_{3,m_j}(0) + e^{i\mu} \sum_{m_j=1}^{N_1} f'_{1,m_j}(0) = 0,
\]

\[
(2.4) \quad f_{2,1}(1) = \cdots = f_{2,N_2}(1) = f_{3,1}(0) = \cdots = f_{3,N_3}(0) = e^{i\mu} f_{1,1}(0) = \cdots = e^{i\mu} f_{1,N_1}(0)
\]

at \( B_n \) in Fig. 3 for each \( n \in \mathbb{Z} \). Then, we obtain a direct integral representation of \( H_k \) such as

\[
U H_k U^{-1} = \int_{[0,2\pi]} H_k(\mu) \frac{d\mu}{2\pi}.
\]

Since \( H_k(\mu) \) acts in the Hilbert space \( \mathcal{H}_\mu \) on the finite graph, the spectrum of \( H_k(\mu) \) is discrete. For \( \mu \in [0,2\pi) \), let \( \{E_n(\mu)\}_{n \in \mathbb{N}} \) be the sequence of the eigenvalues of \( H_k(\mu) \). Assume that \( \{E_n(\mu)\}_{n \in \mathbb{N}} \) are counted with multiplicities and are arranged in the increasing order. Let \( \mathcal{N} \) be the set of natural numbers \( n \) such that \( E_n(\mu) \) does depend on \( \mu \in [0,2\pi) \). Then, we have \( \sigma(H_k) = \sigma_\infty(H_k) \cup \sigma_{ac}(H_k) \), where

\[
\sigma_\infty(H_k) = \bigcup_{n \in \mathcal{N}} \{E_n(\mu)\} \quad \text{and} \quad \sigma_{ac}(H_k) = \bigcup_{n \in \mathcal{N}} \bigcup_{\mu \in [0,2\pi)} \{E_n(\mu)\}.
\]

Seeking an element belonging to \( \sigma(H_k) \setminus \sigma_D(L) \), we pick a \( \lambda \notin \sigma_D(L) \), arbitrarily. For this \( \lambda \), we consider if there exists some \( 0 \neq f = (f_j, m_j)_{j \in \mathcal{J}, m_j = 1, 2, \ldots, N_j} \in \text{Dom}(H_k(\mu)) \) satisfying the characteristic equation \( H_k(\mu)f = \lambda f \). Namely, we consider the system

\[
(2.5) \quad -f''_{j,m_j}(x) + q(x)f_{j,m_j}(x) = \lambda f_{j,m_j}(x)
\]

for \( x \in (0, 1), \ j \in \mathcal{J}, \ m_j = 1, 2, \ldots, N_j \) as well as (2.1), (2.2), (2.3), (2.4). For \( \lambda \in \sigma_D(L) \), a solution to \( -u'' + qu = \lambda u \) is given by

\[
u(x, \lambda) = \theta(x, \lambda) u(0, \lambda) + \frac{\theta(x, \lambda)}{\varphi(1, \lambda)} (u(1, \lambda) - \theta(1, \lambda) u(0, \lambda)). \]
Since \( \sigma_D(L) = \{ \lambda \in R | \varphi(1, \lambda) = 0 \} \), we see that this expression is well-defined. Using (2.2) and (2.4), we see a solution to (2.5) is given by

\[
f_{1,m_1}(x, \lambda) = e^{-i\mu} Y \theta(x, \lambda) + \frac{\varphi(x, \lambda)}{\varphi(1, \lambda)} (X - \theta(1, \lambda)e^{-i\mu} Y), \quad m_1 = 1, 2, \ldots, N_1,
\]

\[
f_{2,m_2}(x, \lambda) = X \theta(x, \lambda) + \frac{\varphi(x, \lambda)}{\varphi(1, \lambda)} (Y - X \theta(1, \lambda)), \quad m_2 = 1, 2, \ldots, N_2,
\]

\[
f_{3,m_3}(x, \lambda) = Y \theta(x, \lambda) + \frac{\varphi(x, \lambda)}{\varphi(1, \lambda)} (s^{-k} X - Y \theta(1, \lambda)), \quad m_3 = 1, 2, \ldots, N_3,
\]

where \( X = f_{1,1}(1) \) and \( Y = f_{2,1}(1) \). Substituting these into (2.1) and (2.3), we derive

\[
-(N_1 \varphi'_1 + N_2 \theta_1 + N_3 \varphi'_3) X + (N_1 e^{-i\mu} + N_2 + s^k N_3) Y = 0,
\]

\[
(N_2 + N_3 s^{-k} + e^{i\mu} N_1) X - (N_1 \theta_1 + N_2 \varphi'_1 + N_3 \theta_1) Y = 0,
\]

where \( \theta_1 = \theta(1, \lambda), \ \theta'_1 = \theta'(1, \lambda), \ \varphi_1 = \varphi(1, \lambda), \ \varphi'_1 = \varphi'(1, \lambda). \) Thus, there exists a non-trivial solution to \( H_k f = \lambda f \) if and only if the determinant of the system on \( X \) and \( Y \) is equal to 0. Putting

\[
M(\lambda, \mu) = \begin{pmatrix}
-N_1 \varphi'_1 + N_2 \theta_1 + N_3 \varphi'_3 & N_1 e^{-i\mu} + N_2 + s^k N_3 \\
N_2 + N_3 s^{-k} + e^{i\mu} N_1 & -(N_1 \theta_1 + N_2 \varphi'_1 + N_3 \theta_1)
\end{pmatrix},
\]

we have

\[
0 = \det M(\lambda, \mu)
\]

\[
= (N_1 + N_3)^2 \theta_1 \varphi'_1 + N_2 (N_1 + N_3) (\varphi'_1)^2 + N_2 (N_1 + N_3) \theta_1^2 + N_2^2 \theta_1 \varphi'_1 \\
- (N_1 N_2 e^{-i\mu} + N_1 N_3 e^{-i\mu} s^{-k} + N_1^2 + N_2^2 + N_2 N_3 s^{-k} + N_1 N_2 e^{i\mu} \\
+ N_2 N_3 s^k + N_3^2 + N_1 N_3 e^{i\mu} s^k).
\]

Since \( \theta_1^2 + (\varphi'_1)^2 = 4A^2 - 2\theta_1 \varphi'_1, \ s^k + s^{-k} = 2 \cos(2\pi k / N) \) and \( e^{-i\mu} s^{-k} + e^{i\mu} s^k = 2 \cos(\mu + (2\pi k / N)) \), we have

\[
0 = \det M(\lambda, \mu)
\]

\[
= (N_1 + N_3)^2 \theta_1 \varphi'_1 + N_2 (N_1 + N_3) (4A^2 - 2\theta_1 \varphi'_1) + N_2^2 \theta_1 \varphi'_1 \\
- \left(2N_1 N_2 \cos \mu + 2N_2 N_3 \cos \frac{2\pi k}{N}\right) + N_1^2 + N_2^2 + N_3^2.
\]
Substituting $\Delta^2 - \Delta_- = \theta_1 \phi_1'$ into this, we obtain

$$0 = \det M(\lambda, \mu)$$

$$= (N_1 + N_2 + N_3)^2 \Delta^2 - (N_1 - N_2 + N_3)^2 \Delta_- - (N_1^2 + N_2^2 + N_3^2)$$

$$- 2 \left( N_1 N_2 \cos \mu + N_2 N_3 \cos \frac{2\pi k}{N} + N_1 N_3 \cos \left( \mu + \frac{2\pi k}{N} \right) \right).$$

Assume that $(N_2 + N_3 \cos(2\pi k/N))^2 + (N_3 \sin(2\pi k/N))^2 \neq 0$. Then, we have

$$N_2 \cos \mu + N_3 \cos \left( \mu + \frac{2\pi k}{N} \right)$$

$$= N_2 \cos \mu + N_3 \left( \cos \mu \cos \frac{2\pi k}{N} - \sin \mu \sin \frac{2\pi k}{N} \right)$$

$$= \left( N_2 + N_3 \cos \frac{2\pi k}{N} \right) \cos \mu - N_3 \sin \frac{2\pi k}{N} \sin \mu$$

$$= \sqrt{\left( N_2 + N_3 \cos \frac{2\pi k}{N} \right)^2 + \left( N_3 \sin \frac{2\pi k}{N} \right)^2} \left( \cos \mu \sin \alpha - \sin \mu \cos \alpha \right)$$

$$= \sqrt{\left( N_2 + N_3 \cos \frac{2\pi k}{N} \right)^2 + \left( N_3 \sin \frac{2\pi k}{N} \right)^2} \sin(\alpha - \mu),$$

where $\alpha$ satisfies

$$\sin \alpha = \frac{1}{\sqrt{(N_2 + N_3 \cos \frac{2\pi k}{N})^2 + (N_3 \sin \frac{2\pi k}{N})^2}} \left( N_2 + N_3 \cos \frac{2\pi k}{N} \right)$$

and

$$\cos \alpha = \frac{1}{\sqrt{(N_2 + N_3 \cos \frac{2\pi k}{N})^2 + (N_3 \sin \frac{2\pi k}{N})^2}} \left( N_3 \sin \frac{2\pi k}{N} \right).$$

Hence, (2.6) implies that

$$2N_1 \sqrt{\left( N_2 + N_3 \cos \frac{2\pi k}{N} \right)^2 + \left( N_3 \sin \frac{2\pi k}{N} \right)^2} \sin(\alpha - \mu)$$

$$= (N_1 + N_2 + N_3)^2 \Delta^2 - (N_1 - N_2 + N_3)^2 \Delta_-$$

$$- \{N_1^2 + (N_2 - N_3)^2\} - 4N_2 N_3 \cos^2 \frac{\pi k}{N}. $$
The eigenvalues for \( H_k(\mu) \) solve this formula, which is called the dispersion relation. The solution \( \lambda \) to (2.7) depends on \( \mu \), thus it generates \( \sigma_{ac}(H_k) \). Since the range of \( \sin(\alpha - \mu) \) is \([-1, 1]\), we have \( \sigma_{ac}(H_k) = \{ \lambda \in \mathbb{R} \mid -1 \leq D(k, \lambda) \leq 1 \} \) and \( \sigma_{\infty}(H_k) = \sigma(D(L)) \).

Next, we assume that \( (N + N_3 \cos(2\pi k/N))^2 + (N_3 \sin(2\pi k/N))^2 = 0. \) Then, we see that (2.6) is equivalent to \( F(k, \lambda) = 0. \) The solution to this equation does not depend on \( \mu \in [0, 2\pi] \). So, we see that \( \sigma_{ac}(H_k) = \emptyset \) and \( \sigma_{\infty}(H_k) = \sigma(D(L)) \cup \{ \lambda \in \mathbb{R} \mid F(k, \lambda) = 0 \} \). \( \square \)

Next, we make preparations for the proof of Theorem 1.3. In the case of \( q = 0 \) and \( k \notin K_0 \), we denote \( D(k, \lambda) \) by \( D_0(k, \lambda) \). Then, we obtain

\[
D_0(k, \lambda) = \frac{(N_1 + N_2 + N_3)^2 \cos^2 \sqrt{\lambda} - \{N_1^2 + (N_2 - N_3)^2\} - 4N_2N_3 \cos^2 \frac{2\lambda}{N}}{2N_1 \sqrt{(N_2 + N_3 \cos \frac{2\lambda}{N})^2 + N_3^2 \sin^2 \frac{2\lambda}{N}}}.
\]

**Lemma 2.1.** For \( k = 0, 1, \ldots, N \), we have the followings:

1. For each \( k \notin K_0 \), the function \( D_0(k, \lambda) \) takes its minimum if and only if \( \cos \sqrt{\lambda} = 0. \) Assume that \( \cos \sqrt{\lambda} = 0. \) Then, we have \( D_0(k, \lambda) \leq 1. \) Moreover, \( D_0(k, \lambda) = -1 \) is equivalent to \( \cos^2(\pi k/N) = (N_1^2 - (N_2 - N_3)^2)/(4N_2N_3) \).

2. For each \( k \notin K_0 \), the function \( D_0(k, \lambda) \) takes its maximum if and only if \( \cos^2 \sqrt{\lambda} = 1. \) Assume that \( \cos^2 \sqrt{\lambda} = 1. \) Then, we have \( D_0(k, \lambda) \geq 1. \) Moreover, \( D_0(k, \lambda) = 1 \) is equivalent to \( k = 0, N \).

**Proof.** Fix \( k \notin K_0 \).

1. It is obvious that \( D_0(k, \lambda) \) takes its minimum if and only if \( \cos \sqrt{\lambda} = 0. \) Assume that \( \cos \sqrt{\lambda} = 0. \) Then, we have

\[
D_0(k, \lambda) = \frac{-N_1^2 + N_2^2 - 2N_2N_3 + N_3^2 + 4N_2N_3 \cos^2 \frac{2\lambda}{N}}{2N_1 \sqrt{N_2^2 + 2N_2N_3 \cos \frac{2\lambda}{N} + N_3^2}} = \frac{-N_1^2 + N_2^2 + 4N_2N_3 \cos^2 \frac{2\lambda}{N} + N_3^2 - 2N_2N_3}{2N_1 \sqrt{N_2^2 + 4N_2N_3 \cos^2 \frac{2\lambda}{N} + N_3^2 - 2N_2N_3}}.
\]

We obtain \( D_0(k, \lambda) \leq -1 \) by utilizing the inequality of arithmetic and geometric means. Moreover, \( D_0(k, \lambda) = -1 \) is valid if and only if \( N_1 = \sqrt{N_2^2 + 4N_2N_3 \cos^2(\pi k/N) + N_3^2 - 2N_2N_3} \), namely \( \cos^2(\pi k/N) = (N_1^2 - (N_2 - N_3)^2)/(4N_2N_3) \).

2. It is obvious that \( D_0(k, \lambda) \) takes its maximum if and only if \( \cos^2 \sqrt{\lambda} = 1. \) Assume that \( \cos^2 \sqrt{\lambda} = 1. \) Then, we have

\[
D_0(k, \lambda) = \frac{N_1N_2 + N_1N_3 + 2N_2N_3(1 - \cos^2 \frac{2\lambda}{N})}{N_1 \sqrt{N_2^2 + N_3^2 + 2N_2N_3(2 \cos^2 \frac{2\lambda}{N} - 1)}}.
\]
Putting \( c = \cos^2(\pi k/N) \in [0,1] \), we consider the function
\[
f(c) = \frac{N_1N_2 + N_1N_3 + 2N_2N_3(1 - c)}{N_1 \sqrt{N_2^2 + N_3^2 + 2N_2N_3(2c - 1)}}.
\]

It follows by straightforward calculations that
\[
f'(c) = -\frac{2N_2N_3(N_2^2 + N_3^2 + 2N_2N_3c + N_1N_2 + N_1N_3)}{N_1 \{N_2^2 + N_3^2 + 2N_2N_3(2c - 1)}^{3/2} < 0
\]
and hence \( f(c) \geq f(1) = 1 \). Thus, we have \( D_0(k, \lambda) \geq 1 \). Moreover, \( D_0(k, \lambda) = 1 \) is equivalent to \( \cos^2(\pi k/N) = 1 \), i.e., \( k = 0, N \).

Recall (1.1). Then, we obtain the followings:

**Lemma 2.2.** Let \( k = 0, 1, 2, \ldots, N \).

1. We see that \( A_+(c, k) \) increases in \( c \in [-1, 1] \) and
   \[
   0 \leq A_+(-1, k) \leq A_+(c, k) \leq A_+(1, k) \leq 1
   \]
   for \( c \in [-1, 1] \). Moreover, \( A_+(1, k) = 1 \) (\( A_+(-1, k) = 0 \), respectively) is equivalent to \( k = 0, N \) (\( \cos^2(\pi k/N) = (N_1^2 - (N_2 - N_3)^2)/(4N_2N_3) \), respectively).

2. We see that \( A_-(c, k) \) decreases in \( c \in [-1, 1] \) and
   \[
   -1 \leq A_-(1, k) \leq A_-(c, k) \leq A_-(1, k) \leq 0
   \]
   for \( c \in [-1, 1] \). Moreover, \( A_-(1, k) = -1 \) (\( A_-(1, k) = 0 \), respectively) is equivalent to \( k = 0, N \) (\( \cos^2(\pi k/N) = (N_1^2 - (N_2 - N_3)^2)/(4N_2N_3) \), respectively).

**Proof.** (1) The monotonicity of \( A_+(c, k) \) and \( A_+(-1, k) \leq A_+(c, k) \leq A_+(1, k) \) are obvious by the definition of \( A_+(c, k) \). Since \( A_+(1, k) \) takes its maximum if and only if \( k = 0, N \), we see that
   \[
   A_+(1, k) \leq A_+(1, 0)
   = \frac{[N_1^2 + N_2^2 - 2N_2N_3 + N_3^2 + 4N_2N_3 + 2N_1 \sqrt{(N_2 - N_3)^2 + 4N_2N_3}]^{1/2}}{N_1 + N_2 + N_3}
   = \frac{[N_1^2 + (N_2 + N_3)^2 + 2N_1(N_2 + N_3)]^{1/2}}{N_1 + N_2 + N_3}
   = 1.
   
   On the other hand, we have
   \[
   A_+(-1, k)
   = \frac{[N_1^2 + (N_2 - N_3)^2 + 4N_2N_3 \cos^2 \frac{\pi k}{N} - 2N_1 \sqrt{(N_2 - N_3)^2 + 4N_2N_3 \cos^2 \frac{\pi k}{N}]^{1/2}}}{N_1 + N_2 + N_3}
   .
   
   (1.1)
Putting \( c = \cos^2(\pi k/N) \in [0, 1] \), we define
\[
g(c) = N_1^2 + (N_2 - N_3)^2 + 4N_2N_3c - 2N_1 \sqrt{(N_2 - N_3)^2 + 4N_2N_3c}.
\]

In the case of \( N_2 = N_3 \) and \( c = 0 \), we have \( g(0) = N_1^2 > 0 \) and hence \( A_+(-1,k) > 0 \). Next, we consider the case where \( (N_2 - N_3)^2 + 4N_2N_3c \neq 0 \). Note that
\[
g'(c) = 4N_2N_3 \left( 1 - \frac{N_1}{\sqrt{(N_2 - N_3)^2 + 4N_2N_3c}} \right).
\]
Assume that there exists \( k \) satisfying \( (N_1^2 - (N_2 - N_3)^2)/(4N_2N_3) = \cos^2(\pi k/N) \). Then \( g(c) \) decreases for \( c \in (0, (N_1^2 - (N_2 - N_3)^2)/(4N_2N_3)) \) and increases for \( c \in ((N_1^2 - (N_2 - N_3)^2)/(4N_2N_3), 1] \). Hence, \( f(c) \geq f((N_1^2 - (N_2 - N_3)^2)/(4N_2N_3)) = 0 \) for \( c \in [0, 1] \).

Next, we consider the case where there does not exist \( k \) satisfying \( (N_1^2 - (N_2 - N_3)^2)/(4N_2N_3) = \cos^2(\pi k/N) \). Then, we claim that \( A_+(-1,k) > 0 \). Assume that \( (N_1^2 - (N_2 - N_3)^2)/(4N_2N_3) < 0 \), which implies \( N_1 < |N_2 - N_3| \). Then, we have \( g'(c) > 0 \) for \( c \in [0, 1] \), and hence \( g(c) \geq g(0) = (N_1 - |N_2 - N_3|)^2 > 0 \) for \( c \in [0, 1] \). Next, we assume that \( (N_1^2 - (N_2 - N_3)^2)/(4N_2N_3) > 1 \), which yields \( N_1 > N_2 + N_3 \). Then, we have \( g'(c) < 0 \) for \( c \in [0, 1] \), and hence \( g(c) \geq g(1) = (N_1 - N_2 - N_3)^2 > 0 \) for \( c \in [0, 1] \). Thus, we see that \( A_+(-1,k) > 0 \) for \( c \in [-1,1] \).

Therefore, \( A_+(-1,k) = 0 \) holds true if and only if there exists \( k \) satisfying \( (N_1^2 - (N_2 - N_3)^2)/(4N_2N_3) = \cos^2(\pi k/N) \). This implies our first claim (1). The second claim is derived because \( A_+(c,k) = -A_-(c,k) \).

**Lemma 2.3.** Fix \( k \notin K_0 \) and \( c \in [-1,1] \). Then, \( D_0(k,\lambda) = c \) if and only if there exists some \( n \in \mathbb{N} \) such that \( \sqrt{\lambda} = 2(n-1)\pi + \arccos A_+(c,k), 2(n-1)\pi + \arccos A_-(c,k), 2(n-1)\pi + 2\pi - \arccos A_+(c,k), 2(n-1)\pi + 2\pi - \arccos A_-(c,k) \in [2(n-1),2n\pi] \).

**Proof.** Since \( D_0(k,\lambda) = c \) is a quadratic equation on \( \cos \sqrt{\lambda} \), we obtain \( \cos \sqrt{\lambda} = A_+(c,k), A_-(c,k) \) as its roots. Since it follows by Lemma 2.2 that \( A_+(c,k) \in [0,1] \) and \( A_-(c,k) \in [-1,0] \), we obtain the desired roots of \( D_0(k,\lambda) = c \).

**Proof of Theorem 1.3.** Due to Lemmas 2.2 and 2.3, we see that \( D_0(k,\lambda) \in [-1,1] \) if and only if there exists some \( j \in \mathbb{N} \) such that \( \sqrt{\lambda} \) belongs to the interval \( [2(j-1)\pi + \arccos A_+(1,k), 2(j-1)\pi + \arccos A_+(-1,k)], [2(j-1)\pi + \arccos A_-(1,k), 2(j-1)\pi + \arccos A_-(1,k)], [2j\pi - \arccos A_+(1,k), 2j\pi - \arccos A_-(1,k)] \). Thus, we obtain the band-gap structure of \( \sigma_{\text{sc}}(H_k) \) described in the statement.
Proof of Theorem 1.5. First, we claim that $0 \notin K_0$. Seeking a contradiction, we assume that $0 \in K_0$. Then, we have $2(N_2^2 + N_3^2) = (N_2 - N_3)^2$, which implies $(N_2 + N_3)^2 = 0$. Thus, we find a contradiction. Since $0 \notin K_0$, we see that $B_j \supset B_j(0)$ for $j \in N$. It follows by $A_+(1, 0) = 1$ and $A_-(1, 0) = -1$ that $\arccos A_+(1, 0) = 0$ and $\arccos A_-(1, 0) = \pi$. Thus, we see that

\begin{align*}
(2.8) \quad & B_{j-3}(0) = \left\{[2(j-1)\pi]^2, 2(j-1)\pi + \arccos A_+(1, k^*)\right\}^2, \\
(2.9) \quad & B_{j-2}(0) = \left\{[2(j-1)\pi + \arccos A_-(1, k^*)]^2, (2j\pi - \pi)^2\right\}, \\
(2.10) \quad & B_{j-1}(0) = \left\{[2(j-1)\pi - \pi]^2, (2j\pi - \arccos A_-(1, k^*)]^2\right\}, \\
(2.11) \quad & B_j(0) = \left\{[2(j-1)\pi - \arccos A_+(1, k^*)]^2, (2j\pi)^2\right\}
\end{align*}

are included in $B_j$. This statement will be used in the following both cases.

(i) Let $K \neq \emptyset$. Then, $k^* \in K$, which implies that $k^* \notin K_0$ and $\cos^2(\pi k^*/N) = (N_1^2 - (N_2 - N_3)^2)/(4N_2N_3)$. Due to Lemma 2.2, we have $A_+(1, k^*) = 0$ and $A_-(1, k^*) = 0$. Thus, we obtain $\arccos A_+(1, k^*) = \arccos A_-(1, k^*) = \pi/2$. Utilizing Theorem 1.3, we obtain

\begin{align*}
B_{j-3}(k^*) &= \left\{[2(j-1)\pi + \arccos A_+(1, k^*)]^2, 2(j-1)\pi + \frac{\pi}{2}\right\}^2, \\
B_{j-2}(k^*) &= \left\{2(j-1)\pi + \frac{\pi}{2}\right\}^2, 2(j-1)\pi + \arccos A_-(1, k^*)\right\}^2, \\
B_{j-1}(k^*) &= \left\{2j\pi - \arccos A_-(1, k^*)\right\}^2, \left(2j\pi - \frac{\pi}{2}\right)^2, \\
B_j(k^*) &= \left\{2j\pi - \frac{\pi}{2}\right\}^2, \left(2j\pi - \arccos A_+(1, k^*)\right\}^2
\end{align*}

If follows by using these formulae, (2.8)–(2.11), and Remark 1.4 that $B_j = B_j(0) \cup B_j(k^*) = \left\{\left[\pi(j-1)/2\right]^2, (\pi j/2)^2\right\}$ for $j \in N$. Thus, we obtain $\sigma_{ac}(H) = [0, \infty)$.

(ii) Assume that $K = \emptyset$. Due to the derivative test in Lemma 2.2, $A_+(1, k)$ attains its minimum for $k$ satisfying $|\cos^2(\pi k/N) - (N_1^2 - (N_2 - N_3)^2)/(4N_2N_3)|$ takes its minimum. Namely, we have $1 > \min_{k \notin K_0} A_+(1, k) = A_+(1, k^*) > 0$. This implies that

\[\frac{\pi}{2} > \max_{k \notin K_0} \arccos A_+(1, k) = \arccos A_+(1, k^*) > 0.\]
Simultaneously, we see that \(-1 < \max_{k \notin k_0} A_{-}(-1, k) = A_{-}(-1, k^*) < 0\) and hence
\[
\frac{\pi}{2} < \min_{k \notin k_0} \arccos A_{-}(-1, k) = \arccos A_{-}(-1, k^*) \leq \pi.
\]
So, we obtain \(B_j = B_j(0) \cup B_j(k^*)\) for \(j \in N\). This combined with Theorem 1.3 yields the result stated in (ii).

We next consider the perturbed case. For sequences \(\{a_n\}_{n=1}^{\infty}\) and \(\{b_n\}_{n=1}^{\infty}\) satisfying \(\inf_{n \in N} |b_n - a_n| \neq 0\) and \(a_n < b_n\) for every \(n \in N\), we define segments
\[
C^{+}(b_n) = \{ \lambda \in C \mid \sqrt{\lambda} = b_n + ti, \ -n \leq t \leq n \},
\]
\[
C^{-}(a_n) = \{ \lambda \in C \mid \sqrt{\lambda} = a_n - ti, \ -n \leq t \leq n \},
\]
\[
C^{\times}(a_n, b_n) = \{ \lambda \in C \mid \sqrt{\lambda} = ni + b_n + t(a_n - b_n), \ 0 \leq t \leq 1 \},
\]
\[
C^{-}(a_n, b_n) = \{ \lambda \in C \mid \sqrt{\lambda} = -ni + a_n + t(b_n - a_n), \ 0 \leq t \leq 1 \}
\]
and the contour \(C(a_n, b_n) = C^{+}(b_n) + C^{\times}(a_n, b_n) + C^{-}(a_n) + C^{-}(a_n, b_n)\) for each \(n \in N\). Moreover, let \(\Omega(a_n, b_n)\) be the region surrounded by \(C(a_n, b_n)\) for each \(n \in N\). The first aim in the perturbed case is to establish the following.

**Lemma 2.4.** Let \(k \notin K_0\).

(I) Fix \(c \in (-1, 1)\). Then, there exists some \(n_0 \in N\) satisfying the followings for all \(n > n_0\):

(i) \(D(k, \lambda) - c\) has exactly one zero inside \(\Omega(2(n - 1)\pi, 2(n - 1)\pi + \pi/2)\).

(ii) \(D(k, \lambda) - c\) has exactly one zero inside \(\Omega(2(n - 1)\pi + \pi/2, 2(n - 1)\pi + \pi)\).

(iii) \(D(k, \lambda) - c\) has exactly one zero inside \(\Omega(2(n - 1)\pi + \pi, 2(n - 1)\pi + 3\pi/2)\).

(iv) \(D(k, \lambda) - c\) has exactly one zero inside \(\Omega(2(n - 1)\pi + 3\pi/2, 2(n - 1)\pi + 2\pi)\).

(v) \(D(k, \lambda) - c\) has exactly 2n zeroes inside \(\Omega(-n\pi, n\pi)\).

(vi) There are no zeroes of \(D(k, \lambda) - c\) except the ones stated in (i)–(v).

(II) Putting \(r = \arccos A_{+}(0, k)\), we have \(r \in (0, \pi/2)\). There exists some \(n_0 \in N\) satisfying the followings for all \(n > n_0\):

(i) \(D(k, \lambda) - 1\) has exactly 2 zeroes inside \(\Omega(n\pi - r, n\pi + r)\).

(ii) \(D(k, \lambda) + 1\) has exactly 2 zeroes inside \(\Omega(n\pi + r, n\pi + (\pi - r))\).

(iii) \(D(k, \lambda) - 1\) has exactly 4n - 1 zeroes inside \(\Omega(-2n\pi - r, 2n\pi - r)\).

(iv) \(D(k, \lambda) + 1\) has exactly 4n zeroes inside \(\Omega(-2n\pi - r, 2n\pi - r)\).

(v) There are no zeroes of \(D(k, \lambda) \pm 1\) except the ones stated in (i)–(iv).

In order to prove this lemma, we prepare lemmas.
Lemma 2.5. We have the followings:

(i) For a fixed $p \in \mathbb{R}$, there exists some constants $C_p > 0$ and $n_0(p) \in \mathbb{N}$ such that $e^{\operatorname{Im} \sqrt{\lambda}} < C_p |\cos \sqrt{\lambda} + p|$ on $C_\pm(n) := \{ \lambda \in \mathbb{C} \mid \sqrt{\lambda} = \pm n + t, t \in \mathbb{R} \}$ for any $n \geq n_0(p)$.

(ii) For a fixed $p \in (-1, 1)$, there exists some constant $C'_p > 0$ such that $e^{\operatorname{Im} \sqrt{\lambda}} < C'_p |\cos \sqrt{\lambda} + p|$ on $C(n, q) := \{ \lambda \in \mathbb{C} \mid \sqrt{\lambda} = n\pi + \arccos q + ti, -n \leq t \leq n \}$ for each $q \in [-1, 1] \setminus \{p, -p\}$ and $n \in \mathbb{N}$.

(iii) For a fixed $p \in \mathbb{R}$, there exists some constant $C''_p > 0$ such that $e^{\operatorname{Im} \sqrt{\lambda}} < C''_p |\cos \sqrt{\lambda} + p|$ on $C(n, q)$ for each $q \in (-1, 1) \setminus \{p, -p\}$ and $n \in \mathbb{N}$.

The proof of Lemma 2.5 is found in [13, Lemma 3.6 and Remark 3.7].

Lemma 2.6. Let $k \notin K_0$. We have

$$D(k, \lambda) = D_0(k, \lambda) + o\left(\frac{e^{2\operatorname{Im} \sqrt{\lambda}}}{|\sqrt{\lambda}|}\right) \quad \text{as} \quad |\lambda| \to \infty.$$ 

Especially, we obtain

$$\lim_{\lambda \to -\infty} D(k, \lambda) = +\infty.$$ 

Proof. From [17], we quote the asymptotic result as $|\lambda| \to \infty$ of the fundamental solutions:

$$\theta(1, \lambda) = \cos \sqrt{\lambda} + \frac{1}{2\sqrt{\lambda}} \int_0^1 (\sin \sqrt{\lambda} + \sin \sqrt{\lambda}(1 - 2t))q(t)dt + o\left(\frac{e^{2\operatorname{Im} \sqrt{\lambda}}}{|\lambda|}\right),$$

$$\varphi'(1, \lambda) = \cos \sqrt{\lambda} + \frac{1}{2\sqrt{\lambda}} \int_0^1 (\sin \sqrt{\lambda} + \sin \sqrt{\lambda}(1 - 2t))q(t)dt + o\left(\frac{e^{2\operatorname{Im} \sqrt{\lambda}}}{|\lambda|}\right).$$

These formulae yield

$$A^2(\lambda) = \cos^2 \sqrt{\lambda} + o\left(\frac{e^{2\operatorname{Im} \sqrt{\lambda}}}{|\sqrt{\lambda}|}\right) \quad \text{and} \quad \tilde{A}^2(\lambda) = o\left(\frac{e^{2\operatorname{Im} \sqrt{\lambda}}}{|\sqrt{\lambda}|}\right)$$

as $|\lambda| \to \infty$. Substituting these into the definition of $D(k, \lambda)$, we obtain our desired formula.

Proof of Lemma 2.4. (I) Let $c \in (-1, 1)$. Then, we see that $0 < A_+(c, k) < 1$ and $-1 < A_-(c, k) < 0$ because of Lemma 2.2. Utilizing Lemma 2.5 (i) and (ii), there exists some constant $C = C(c, k) > 0$ and $n_0 = n_0(c, k) \in \mathbb{N}$ such that

$$e^{2\operatorname{Im} \sqrt{\lambda}} < C |\cos \sqrt{\lambda} - A_+(c, k)||\cos \sqrt{\lambda} - A_-(c, k)|$$

(2.13)
on each contour $C(2(n-1)\pi, 2(n-1)\pi + \pi/2)$, $C(2(n-1)\pi + \pi/2, 2(n-1)\pi + \pi)$, $C(2(n-1)\pi + \pi, 2(n-1)\pi + 3\pi/2)$, $C(2(n-1)\pi + 3\pi/2, 2(n-1)\pi + 2\pi)$ and $C(-n\pi, n\pi)$ for $n \geq n_0$. When we use Lemma 2.5 (ii) here, we put $p = A_+(c,k), A_-(c,k)$ and can take $q = 1, -1, 0$. Then, we obtain (2.13) because $\arccos q = 0, \pi, \pi/2$.

Since $A_+(c,k)$ and $A_-(c,k)$ play the role of roots for $D_0(k, \lambda) = c$, we have

$$D_0(k, \lambda) - c = M(N_1, N_2, N_3, k)(\cos \sqrt{\lambda} - A_+(c,k))(\cos \sqrt{\lambda} - A_-(c,k)),$$

where

$$M(N_1, N_2, N_3, k) := \frac{(N_1 + N_2 + N_3)^2}{2N_1 \sqrt{(N_2 + N_3 \cos \frac{2\pi k}{N})^2 + N_3^2 \sin^2 \frac{2\pi k}{N}}} > 0.$$

Hence, we obtain

$$|(D(k, \lambda) - c) - (D_0(k, \lambda) - c)| = \theta \left(\frac{1}{\sqrt{\lambda}}\right) |D_0(k, \lambda) - c|$$

as $|\lambda| \to \infty$ on the above 5 types of contours because of Lemma 2.6 and (2.13). Utilizing the Rouché’s theorem, we see that the number of zeroes of $D(k, \lambda) - c$ is the same as the one for $D_0(k, \lambda) - c$ inside each region $\Omega(2(n-1)\pi, 2(n-1)\pi + \pi/2)$, $\Omega(2(n-1)\pi + \pi/2, 2(n-1)\pi + \pi)$, $\Omega(2(n-1)\pi + \pi, 2(n-1)\pi + 3\pi/2)$, $\Omega(2(n-1)\pi + 3\pi/2, 2(n-1)\pi + 2\pi)$ and $C(-n\pi, n\pi)$ for a large $n \in \mathbb{N}$. The number of zeroes of $D_0(k, \lambda) - c$ can be counted by using Lemma 2.2.

(II) Thanks to Lemma 2.2, we have $0 < A + (0, k) < 1$ and $-1 < A_-(0, k) < 0$. Thus, we obtain $r \in (0, \pi/2)$. Moreover, we utilize Lemma 2.5 (i) and (iii) as $p = 1$ and $q = A_-(0, k), A_+(0, k)$. Since $r = \arccos A_+(0, k)$ and $\pi - r = \arccos A_-(0, k)$, we have the same estimate as (2.13) on each contour $C(n \pi - r, n \pi + r)$, $C(n \pi + r, n \pi + (\pi - r))$, $C(-(2n \pi - r), (2n \pi - r))$ and $C(-(2n \pi - r), 2n \pi - r)$ for a large $n \in \mathbb{N}$. In a similar way to (I), we obtain the statement (II).

Before we start the proof of Theorem 1.8, we need the further lemmas.

**Lemma 2.7.** Let $k \notin K_0$.

1. Assume that $A(\lambda) = 0$. Then, we have $D(k, \lambda) \leq -1$.
   a. If $K = \emptyset$, then $D(k, \lambda) < -1$.
   b. If $K \neq \emptyset$, then $D(k, \lambda) < -1$ for $k \neq k^*, N - k^*$.

2. Assume that $\lambda \in \sigma_D(L)$. Then, we have $D(k, \lambda) \geq 1$. If $k \neq 0, N$, then $D(k, \lambda) > 1$. 


Proof. (1) It follows by straightforward calculations that
\[
D(k, \lambda) = -\frac{(N_1 - N_2 + N_3)^2}{2N_1 \sqrt{N_2^2 + 4N_2N_3 \cos^2 \frac{\pi k}{N}}} + \lambda^2 + D_1(k, \lambda),
\]
where
\[
D_1(k, \lambda) = \frac{(N_1 + N_2 + N_3)^2 \lambda^2 - \{N_1^2 + (N_2 - N_3)^2\} - 4N_2N_3 \cos^2 \frac{\pi k}{N}}{2N_1 \sqrt{N_2^2 + 4N_2N_3 \cos^2 \frac{\pi k}{N}}}.
\]
In a similar way to (the proof of) Lemma 2.1, we see that \(D_1(k, \lambda) \leq -1\). Furthermore, we see that \(D_1(k, \lambda) = -1\) if and only if \(K \neq \emptyset\) and \(k = k^*\), \(N - k^*\). Thus, we obtain the first statement.

(2) For \(\lambda \in \sigma_D(L)\), we have \(\varphi_1 = 0\). Thus, we obtain \(\theta_1 \varphi_1' = 1\). Since \(A^2 - A_2^2 = \theta_1 \varphi_1'\), we derive \(-A_2^2 = 1 - A^2\). So, we obtain
\[
2N_1 \sqrt{N_2^2 + 4N_2N_3 \cos^2 \frac{\pi k}{N}} + N_3^2 - 2N_2N_3D(k, \lambda)
\]
\[
= [(N_1 + N_3)^2 + 2N_2(N_1 + N_3) + N_2^2
- \{(N_1 + N_3)^2 - 2N_2(N_1 + N_3) + N_2^2\}]A^2
+N_1^2 - 2N_1(N_2 - N_3) + (N_2 - N_3)^2 - N_1^2
- (N_2 - N_3)^2 - 4N_2N_3 \cos^2 \frac{\pi k}{N}
\]
\[
= 4N_2(N_1 + N_3)A^2 - 2N_1(N_2 - N_3) - 4N_2N_3 \cos^2 \frac{\pi k}{N}
\]
\[
\geq 4N_1N_2 + 4N_2N_3 - 2N_1N_2 + 2N_1N_3 - 4N_2N_3 \cos^2 \frac{\pi k}{N}
\]
\[
= 2 \left\{N_1N_2 + N_1N_3 + 2N_2N_3 \left(1 - \cos^2 \frac{\pi k}{N}\right)\right\}.
\]
Here, we used \(A^2 \geq 1\), which is valid because \(\lambda \in \sigma_D(L)\) is located in the closure of spectral gap of \(L\). Thus, we have \(D(k, \lambda) > D_0(k, \lambda) \geq 1\) by virtue of (the proof) of Lemma 2.1. Since \(D_0(k, \lambda) = 1\) is equivalent to \(k = 0, N\), we obtain the second statement. \(\square\)

Recall \(r = \arccos A_+(0, k)\) and \(\sigma_D(L) = \{\mu_n\}_{n=1}^{\infty}\). Furthermore, we define \(\mu_0 = \min\{\lambda \in \mathbb{R} | A(\lambda) = 1\}\). Let \(\{\eta_n\}_{n=1}^{\infty}\) be the set of zeroes of \(A(\lambda)\), which is arranged in the increasing order. Since the behavior of the spectral discriminant is well-known, we see that \(\mu_0 < \eta_1 < \mu_1 < \eta_2 < \mu_2 < \cdots\).
Lemma 2.8. There exists some \( n_0 \in \mathbb{N} \) satisfying the followings for \( n \geq n_0 \):

(i) \( \mu_0, \mu_1, \ldots, \mu_{2n-1} \) is belonging to the interval \((-2\pi n - r)^2, (2\pi n - r)^2\).

(ii) \( \eta_1, \eta_2, \ldots, \eta_{2n} \) is belonging to the interval \((-2\pi n - r)^2, 2\pi n - r\).

(iii) \( \mu_n \) is belonging to the interval \((n\pi - r)^2, (n\pi + r)^2\).

(iv) \( \eta_{n+1} \) is belonging to the interval \((n\pi + r)^2, (n\pi + (\pi - r))^2\).

Proof. Although this lemma is a classical result, we give a proof in short. Recall \( \mu_n \in [\lambda_{2n-1}, \lambda_{2n}] \) for \( n \in \mathbb{N} \), where \( (\lambda_{2n-1}, \lambda_{2n}) \) be the \( n \)th spectral gap of \( L \). Furthermore, we have \( \Delta(\lambda) = \cos \sqrt{\lambda} + \mathcal{O}(1/\sqrt{\lambda}) \) as \( \lambda \to +\infty \). Thus, it follows by Rouché’s theorem that \( \mu_n \) is close to \( n^2\pi^2 \) for a large \( n \in \mathbb{N} \). In a similar way, \( \eta_{n+1} \) is close to \( (n\pi + \pi/2)^2 \) for a large \( n \in \mathbb{N} \).

Proof of Theorem 1.8. Due to Lemma 2.4 (II), there are \( \lambda_{k,0}^+, \lambda_{k,2}^-, \lambda_{k,2}^+, \ldots, \lambda_{k,4n-2}^+, \lambda_{k,4n-2}^- \) as the \((4n-1)\) zeroes of \( D(k, \lambda) - 1 \) inside \( \Omega(-2\pi n, -2\pi n - r) \) for a large \( n \in \mathbb{N} \). In a similar way, there are \( \lambda_{k,0}^-, \lambda_{k,1}^-, \lambda_{k,1}^+, \lambda_{k,3}^-, \lambda_{k,3}^+, \ldots, \lambda_{k,4n-1}^-, \lambda_{k,4n-1}^+ \) as the \( 4n \) zeroes of \( D(k, \lambda) + 1 \) inside \( \Omega(-2\pi n, 2\pi n - r) \) for a large \( n \in \mathbb{N} \). According to Lemma 2.8, we have \( \mu_0, \mu_1, \ldots, \mu_{2n-1} \in (-2\pi n - r)^2, (2\pi n - r)^2 \) and \( \eta_1, \eta_2, \ldots, \eta_{2n} \in (-2\pi n - r)^2, (2\pi n - r)^2 \) for a large \( n \in \mathbb{N} \). Moreover, it follows by Lemma 2.7 that \( D(k, \mu_p) \geq 1 \) for \( p = 0, 1, 2, \ldots, 2n \) and \( D(k, \eta_p) \leq -1 \) for \( p = 0, 1, 2, \ldots, 2n \). Thus, we see that \( \lambda_{k,0}^+, \lambda_{k,2}^-, \lambda_{k,2}^+, \ldots, \lambda_{k,4n-2}^+, \lambda_{k,4n-2}^- \) and \( \lambda_{k,1}^-, \lambda_{k,1}^+, \lambda_{k,3}^-, \lambda_{k,3}^+, \ldots, \lambda_{k,4n-1}^-, \lambda_{k,4n-1}^+ \) are real due to Lemma 2.4 (I) and (2.12). Furthermore, it follows by \( \mu_0 < \eta_1 < \mu_1 < \eta_2 < \cdots < \mu_{2n-1} < \eta_{2n} \) that

\[
\lambda_{k,0}^+ < \lambda_{k,1}^- \leq \lambda_{k,1}^+ < \lambda_{k,2}^- \leq \lambda_{k,2}^+ < \cdots < \lambda_{k,4n-1}^- \leq \lambda_{k,4n-1}^+ < \lambda_{k,4n-2}^- \leq \lambda_{k,4n-2}^+.
\]

Since \( n \) can be taken as a large number, we obtain (1.2) and \( \sigma_{ac}(H_k) = \bigcup_{j=1}^{n} [\lambda_{k,j-1}, \lambda_{k,j}] \). Furthermore, we obtain the statement (A), (B), and (C) by virtue of Lemma (1)-(a),(b) and (2). The inequality in (D) holds true because of Lemma 2.7.

Proof of Theorem 1.10. Since \( q \) is even, we have \( \Delta(\lambda) = \theta(1, \lambda) = \varphi'(1, \lambda) \) and hence \( \Delta(\lambda) = 0 \). On the other hand, there exists some \( j \in \mathbb{N} \) and \( \lambda \in [\lambda_{2j-1}, \lambda_{2j}] \) such that \( \Delta^2(\lambda) > 1 \) because \( q \) is a gap-opening potential. We fix \( k = 0, 1, \ldots, N \), arbitrarily. For this \( \lambda \), we can assume that \( \lambda \notin \sigma_{\infty}(H) \) because \( \sigma_{\infty}(H) \) is discrete. Under these preparations, we have

\[
2N_1 \sqrt{N_2^2 + 4N_2N_3 \cos^2 \frac{\pi k}{N}} + N_3^2 - 2N_2N_3 D(k, \lambda) > (N_1 + N_2 + N_3)^2 - \{N_1^2 + (N_2 - N_3)^2\} - 4N_2N_3 \cos^2 \frac{\pi k}{N}
\]

\[
= 2 \left\{ N_1N_2 + N_1N_3 + 2N_2N_3 \left( 1 - \cos^2 \frac{\pi k}{N} \right) \right\}.
\]
Since we have already proved that
\[
\left\{ \frac{N_1 N_2 + N_1 N_3 + 2N_2 N_3 (1 - \cos^2 \frac{\pi}{N})}{N_1 \sqrt{N_2^2 + 4N_2 N_3 \cos^2 \frac{\pi}{N} + N_3^2 - 2N_2 N_3}} \right\}
\]
is greater than or equal to 1, we obtain \( D(k, \lambda) > 1 \) for \( \lambda \) and any combination of \( N_1, N_2, N_3 \). Let \( \eta_1 \) be the first zero of \( A(\lambda) \). Since \( \eta_1 \leq \lambda \) and \( D(k, \eta_1) \leq -1 \), we have \( \lambda \in [\lambda^+_k, \infty) \). Thus, we see that this \( \lambda \) is a spectral gap.

\[\square\]

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