Schrödinger Operators on a Zigzag Supergraphene-Based Carbon Nanotube

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Abstract. Throughout this paper, we study the spectrum of a periodic Schrödinger operator on a zigzag super carbon nanotube, which is a generalization of the zigzag carbon nanotube. We prove that its absolutely continuous spectrum has the band structure. Moreover, we show that its eigenvalues with infinite multiplicities consisting of the Dirichlet eigenvalues and points embedded in the spectral band for some corresponding Hill operator. We also give the asymptotics for the spectral band edges.

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1 Introduction

The Royal Swedish Academy of Sciences has awarded the Nobel Prize in Physics for 2010 to A. Geim and K. Novoselov for groundbreaking experiments regarding the two-dimensional material graphene (Fig. 1). Graphene is a thin monolayer of pure carbons located in the vertexes of the hexagonal lattice. Although its thickness is a single atom size, graphene is also known as the strongest materials. Moreover, graphene has outstanding properties on the thermal and electrical conduction and tribology. Thus, graphene nowadays plays important roles in the field of mechanical engineering. These days, mathematicians are also interested in the spectral theory for differential and difference Schrödinger operators on the metric and discrete graph corresponding to materials with nanostructures. As stated in the opening paragraph of [3], researchers recently are suggesting new models of two-dimensional carbon allotropes and studying its properties as materials before they are synthesized. Graphene-like models are called graphynes. Do
and Kuchment [3] studied the dispersion relations and spectra of Schrödinger operators on one of graphynes, namely, the 2-dimensional lattice consisting of hexagons and rhombuses. In the dispersion relation, they found spectral gaps and conical Dirac points, which are important in the theory of the solid state physics, especially in that of topological insulators. The motivation of [3] originated from the paper [4] by chemists. Enyashin and Ivanovski suggested 14 types of graphynes in their paper [4]. Their paper includes the results of dispersion relation. From the view point of quantum graphs, there are spectral results for graphyne and its nanotubes consisting of hexagons and rhombuses [2, 3]. In the graphynes appearing in [4], we also find supergraphene (see also [20]). According to the paper [20], it reads that supergraphene is formed when the carbon-carbon bonds in graphene are completely replaced by carbine-like chains (Fig. 1).

Throughout this paper, we construct the spectral theory of Schrödinger operators on a supergraphene-based carbon nanotube. Standard carbon nanotubes are graphene sheets with a cylindrical structure (Fig. 2). Single-wall carbon nanotubes are classified into three classes: zigzag, armchair and chiral. The spectral theory for Schrödinger operators on the graphene and the carbon nanotubes are constructed in [10, 12]. In this paper, we suggest a new supergraphene-based zigzag carbon nanotube, which can be called a zigzag super carbon nanotube, and study its spectral properties by a quantum graph approach [1].

Let us define a metric graph $\Gamma^N$ corresponding to zigzag super carbon nanotube (Fig. 2) for a fixed $N \in \mathbb{N}$. We put $J = \{1, 2, 3, 4, 5, 6, 7, 8, 9\}$, $e_0 = (0, 0, 1)$, $Z_N = \mathbb{Z} / (N\mathbb{Z}) = \{0, 1, 2, \cdots, N-1\}$ and $R_N = \frac{\sqrt{3}}{4\sin \frac{\pi}{N}}$. For $k \in Z_N$, let $c_k = \cos \frac{nk}{N}$, $s_k = \sin \frac{nk}{N}$ and $k_k = R_N(c_k, s_k, 0)$. For $\omega = (n, j, k) \in Z := \mathbb{Z} \times J \times Z_N$, we define the edge $\Gamma_\omega = \{x = 3r_\omega + te_\omega \mid t \in [0, 1]\}$, where

- $e_{n,1,k} = e_{n,2,k} = e_{n,3,k} = e_0$, $e_{n,4,k} = e_{n,5,k} = e_{n,6,k} = k_n + 2k + 1 - k_n + 2k + \frac{e_0}{2}$,
- $e_{n,7,k} = e_{n,8,k} = e_{n,9,k} = -\left(k_n + 2k + 2 - k_n + 2k + 1 - \frac{e_0}{2}\right)$,
- $r_{n,1,k} = k_n + 2k + \frac{3n}{2}e_0$, $r_{n,2,k} = r_{n,1,k} + \frac{1}{3}e_{n,1,k}$, $r_{n,3,k} = r_{n,2,k} + \frac{1}{3}e_{n,2,k}$,
- $r_{n,4,k} = r_{n,1,k} + e_0$, $r_{n,5,k} = r_{n,4,k} + \frac{1}{3}e_{n,4,k}$, $r_{n,6,k} = r_{n,5,k} + \frac{1}{3}e_{n,5,k}$,
- $r_{n,7,k} = r_{n+1,0,k} - e_{n,7,k}$, $r_{n,8,k} = r_{n+1,0,k} - \frac{2}{3}e_{n,7,k}$, $r_{n,9,k} = r_{n+1,0,k} - \frac{1}{3}e_{n,7,k}$.

Fig. 1: Graphene (left) and supergraphene (right).
Taking the union $\Gamma^N := \bigcup_{\omega \in \mathbb{Z}} \Gamma_\omega$, we obtain the cylindrical metric graph seen in the right picture in Fig. 2, which is the case of $N = 8$. Cutting and opening $\Gamma^N$ in order to understand the notation $\Gamma_\omega$, we obtain a part of the graphene sheet as in Fig. 3.

We next define a quantum graph for a zigzag super carbon nanotube. Namely, we define a periodic Schrödinger operator on each edge $\Gamma_{n,j,k}$ and a vertex condition. First, we abbreviate $y_\omega = y|_{\Gamma_\omega}$ for a function $y$ defined on $\Gamma^N$ and $\omega \in \mathbb{Z}$. Moreover, we identify every edge $\Gamma_\omega$ as the interval $[0,1]$ and give the local coordinate $x \in [0,1]$. We consider the
Hilbert space $L^2(\Gamma^N) = \bigoplus_{\omega \in \mathbb{Z}} L^2(\Gamma_\omega)$ equipped with the inner product
\[
\langle \psi, \varphi \rangle_{L^2(\Gamma^N)} = \sum_{\omega \in \mathbb{Z}} \langle \psi_\omega, \varphi_\omega \rangle_{L^2(\Gamma_\omega)} \quad \text{for} \quad \psi = \{\psi_\omega\} \omega \in \mathbb{Z}, \quad \varphi = \{\varphi_\omega\} \omega \in \mathbb{Z} \in L^2(\Gamma^N).
\]

Let $\Gamma_\omega^0$ be the interior of $\Gamma_\omega$. For a real-valued function $q \in L^2(0,1)$, we define
\[
(Hf_\omega)(x) = -f'''_\omega(x) + q(x)f_\omega(x), \quad x \in (0,1) \simeq \Gamma_\omega^0, \quad \omega \in \mathbb{Z},
\]

\[
\text{Dom}(H) = \bigoplus_{\omega \in \mathbb{Z}} f_\omega \in L^2(\Gamma^N)
\]

where $f'_\omega(1)$ and $f'_\omega(0)$ imply $f_\omega'(1) = 0$ and $f_\omega'(0)$ for $\omega \in \mathbb{Z}$. Here, $\bigoplus_{\omega \in \mathbb{Z}} (-f'''_\omega + qf_\omega) \in L^2(\Gamma^N)$ also implies that $f_\omega$ and $f'_\omega$ are absolutely continuous on each interval $\Gamma_\omega^0$. At each vertex, the Kirchhoff condition [11] is imposed. The boundary condition is also called the free boundary condition or the Neumann vertex condition. This boundary condition implies that any function $y \in \text{Dom}(H)$ is continuous on $\Gamma^N$ and satisfies the zero flux condition at each vertex of $\Gamma^N$. Self-adjointness of $H$ has already been established in [16].

Utilizing the same method as [10, Theorem 1.1], we obtain the unitarily equivalence between our Hamiltonian $H$ and the direct sum of $N$ operators on the degenerate zigzag super carbon nanotube $\Gamma^1$ (see Fig. 4). Let us describe the definition of the $N$ operators. For convenience, we abbreviate $\Gamma_{n,j} = \Gamma_{n,j}$ for $(n,j) \in \mathbb{Z} \times \mathbb{J}$. For a fixed $N \in \mathbb{N}$, we
put \( s = e^{i\frac{2\pi}{N}} \). For \( k = 1,2,\cdots,N \), we consider the operator \( H_k \) in \( L^2(\Gamma^1) \) defined as
\[
(H_k f_{n,j})(x) = -u''_{n,j}(x) + q(x)u_{n,j}(x), \quad x \in (0,1) \cong \Gamma^1, \quad (n,j) \in \mathcal{Z}_1 := \mathbb{Z} \times \mathbb{J},
\]
\[
\text{Dom}(H_k) = \bigoplus_{(n,j) \in \mathcal{Z}_1} u_{n,j} \in L^2(\Gamma^1)
\]
\[
\bigoplus_{(n,j) \in \mathcal{Z}_1} \left( -u''_{n,j} + qu_{n,j} \right) \in L^2(\Gamma^1),
\]
\[
\begin{align*}
&u_{n,1}(1) = u_{n,2}(0), \quad u'_{n,1}(1) = u'_{n,2}(0), \\
&u_{n,2}(1) = u_{n,3}(0), \quad u'_{n,2}(1) = u'_{n,3}(0), \\
&u_{n,3}(1) = u_{n,4}(0) = s^k u_{n,7}(0), \\
&-u'_{n,3}(1) + u'_{n,4}(0) + s^k u'_{n,7}(0) = 0, \\
&u_{n,4}(1) = u_{n,5}(0), \quad u'_{n,4}(1) = u'_{n,5}(0), \\
&u_{n,5}(1) = u_{n,6}(0), \quad u'_{n,5}(1) = u'_{n,6}(0), \\
&u_{n,6}(1) = u_{n,7}(0), \quad u'_{n,6}(1) = u'_{n,7}(0), \\
&u_{n,7}(1) = u_{n,8}(0), \quad u'_{n,7}(1) = u'_{n,8}(0), \\
&u_{n,8}(1) = u_{n,9}(0), \quad u'_{n,8}(1) = u'_{n,9}(0), \\
&u_{n,9}(1) = u_{n,10}(0), \quad u'_{n,9}(1) = u'_{n,10}(0), \\
&-u'_{n,10}(1) + u'_{n,11}(0) + u'_{n+1,1}(0) = 0
\end{align*}
\]

Since we see that \( H \) unitarily equivalent to \( \bigoplus_{k=1}^N H_k \) in a similar way to [10, Theorem 1.1], we have
\[
\sigma(H) = \bigcup_{k=1}^N \sigma(H_k).
\]

Thus, we examine \( \sigma(H_1), \sigma(H_2), \cdots, \sigma(H_N) \) throughout this paper. We put \( H_0 = H_N \).

In order to describe our first theorem, we need notations related to the classical spectral theory for the Hill operator \( L := -d^2/dx^2 + q \) in \( L^2(\mathbb{R}) \), where the potential \( q \) of the Hamiltonian \( H \) is extended to the periodic function on \( \mathbb{R} \) with the period 1. Let \( \theta(x,\lambda) \) and \( \varphi(x,\lambda) \) be the solutions to the Schrödinger equation
\[
-\varphi''(x,\lambda) + q(x)\varphi(x,\lambda) = \lambda \varphi(x,\lambda), \quad x \in \mathbb{R}, \quad \lambda \in \mathbb{C}
\]
(1.1)
as well as the initial conditions \( \theta(0,\lambda) = 1, \theta'(0,\lambda) = 0 \) and \( \varphi(0,\lambda) = 0, \varphi'(0,\lambda) = 1 \), respectively. Since \( \theta(x,\lambda), \theta'(x,\lambda), \varphi(x,\lambda), \varphi'(x,\lambda) \) are entire in \( \lambda \in \mathbb{C} \), the Lyapunov function
\[
\Delta(\lambda) := \frac{\theta(1,\lambda) + \varphi'(1,\lambda)}{2}
\]
is also entire in \( \lambda \in \mathbb{C} \). It is known as the Floquet–Bloch theory [13, 19] that the spectrum of \( L \) is characterized by \( \Delta(\lambda) \) as
\[
\sigma(L) = \sigma_{ac}(L) = \left\{ \lambda \in \mathbb{R} \mid -1 \leq \Delta(\lambda) \leq 1 \right\} = \bigcup_{j \in \mathbb{N}} [\lambda_{2j-2}, \lambda_{2j-1}],
\]
where \( \lambda_0, \lambda_3, \lambda_4, \lambda_7, \lambda_8, \cdots \) are zeroes of \( \Delta(\lambda) - 1 \), \( \lambda_1, \lambda_2, \lambda_5, \lambda_6, \cdots \) are zeroes of \( \Delta(\lambda) + 1 \) and they are labeled in the increasing order. These zeroes satisfy the inequality
\[
\lambda_0 < \lambda_1 < \lambda_2 < \lambda_3 < \cdots
\]
\[ \lambda_3 \leq \lambda_4 < \cdots \] For \( j \in \mathbb{N} \), the interval \( B_j := [\lambda_{2j-2}, \lambda_{2j-1}] \) is called the \( j \)-th band of \( \sigma(L) \), counted from the bottom. Two consecutive bands \( B_j \) and \( B_{j+1} \) are separated by \( G_j := (\lambda_{2j-1}, \lambda_{2j}) \), which is referred as the \( j \)-th gap of \( \sigma(L) \). 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 put \( \sigma^D(L) = \{ \mu_n \}_{n=1}^{\infty} \), where \( \{ \mu_n \}_{n=1}^{\infty} \) is arranged in the increasing order.

Then, we have \( \sigma^D(L) = \{ \lambda \in \mathbb{R} | \varphi(1, \lambda) = 0 \} \) and \( \mu_n \in [\lambda_{2n-1}, \lambda_{2n}] \) for each \( n \in \mathbb{N} \) (see [18]).

Using the notations for the Hill operator \( H \), we define the discriminant for our operator \( H_k \). We put \( \Delta_{-} = \sqrt{\vartheta'(1, \lambda) - \vartheta(1, \lambda)} \). If \( (N, k) \neq (2\ell, \ell) \) for any \( \ell \in \mathbb{N} \), then we define

\[
D(k, \lambda) = \frac{1}{4 \cos^2 \pi \frac{k}{N}} \left\{ 144\Delta^6 - (216 + 16\Delta^2)\Delta^4 + (81 + 8\Delta^2)\Delta^2 - (3 + s^k + s^{-k} + \Delta^2) \right\}. \tag{1.2}
\]

In the case where \( N \) is odd, we notice that \( \cos \frac{2\pi k}{N} \neq 0 \) for any \( k = 1, 2, \ldots, N \). Thus, (1.2) is well-defined in the case. If there exists some \( \ell \in \mathbb{N} \) such that \( (N, k) = (2\ell, \ell) \), then we define

\[
D(\ell, \lambda) = D \left( \frac{N}{2}, \lambda \right) = 144\Delta^6 - (216 + 16\Delta^2)\Delta^4 + (81 + 8\Delta^2)\Delta^2 - (1 + \Delta^2).
\]

Furthermore, we define the sets \( \sigma_{1/2}(L) = \{ \lambda \in \mathbb{R} | \Delta = \frac{1}{2} \} \) and \( \sigma_{-1/2}(L) = \{ \lambda \in \mathbb{R} | \Delta = -\frac{1}{2} \} \). Moreover, let \( \sigma_{\infty}(H) \) and \( \sigma_{ac}(H) \) be the set of eigenvalues of \( H \) with infinite multiplicities and the absolutely continuous spectrum of \( H \). Then, we have the followings:

**Theorem 1.1.** (i) Put \( N = 2\ell - 1 \) for a fixed \( \ell \in \mathbb{N} \). Then, we have \( \sigma(H_k) = \sigma_{\infty}(H_k) \cup \sigma_{ac}(H_k) \) for \( k = 1, 2, \ldots, N \), where

\[
\sigma_{\infty}(H_k) = \sigma_{1/2}(L) \cup \sigma_{-1/2}(L) \cup \sigma_D(L) \quad \text{and} \quad \sigma_{ac}(H_k) = \{ \lambda \in \mathbb{R} | -1 \leq D(k, \lambda) \leq 1 \}.
\]

(ii) Put \( N = 2\ell \) for a fixed \( \ell \in \mathbb{N} \). Then, we have \( \sigma(H_k) = \sigma_{\infty}(H_k) \cup \sigma_{ac}(H_k) \) for \( k = 1, 2, \ldots, N \), where

\[
\sigma_{\infty}(H_k) = \begin{cases} \sigma_{1/2}(L) \cup \sigma_{-1/2}(L) \cup \sigma_D(L) & \text{if } k \in \{1, 2, \ldots, N\} \setminus \{N/2\}, \\ \sigma_{1/2}(L) \cup \sigma_{-1/2}(L) \cup \sigma_D(L) \cup \{ \lambda \in \mathbb{R} | D(\ell, \lambda) = 0 \} & \text{if } k = N/2, \end{cases}
\]

and

\[
\sigma_{ac}(H_k) = \begin{cases} \{ \lambda \in \mathbb{R} | -1 \leq D(k, \lambda) \leq 1 \} & \text{if } k \in \{1, 2, \ldots, N\} \setminus \{N/2\}, \\ \emptyset & \text{if } k = N/2. \end{cases}
\]

On the absolutely continuous spectrum of \( H_k \), we have the followings:

**Theorem 1.2.** (i) For \( k = 0, 1, 2, \ldots, N \), we have \( \sigma_{ac}(H_k) = \sigma_{ac}(H_{N-k}) \). Hence, we have

\[
\sigma_{ac}(H) = \bigcup_{k=0}^{N-1} \sigma_{ac}(H_k)
\]
in the both case of \( N = 2\ell - 1 \) and \( N = 2\ell \) for a fixed \( \ell \in \mathbb{N} \).

(ii) Let \( N = 2\ell - 1 \) or \( N = 2\ell \) for a fixed \( \ell \in \mathbb{N} \). For \( k = 0, 1, 2, \cdots, \ell - 1 \), there exists real sequence

\[
\lambda_{k,0}^- < \lambda_{k,1}^- < \lambda_{k,1}^+ < \lambda_{k,2}^- < \cdots < \lambda_{k,n}^- < \lambda_{k,n}^+ < \cdots
\]
such that \( \sigma_{ac}(H_k) = \bigcup_{j=1}^\infty [\lambda_{k,j-1}^+, \lambda_{k,j}^-] \). Namely, \( \sigma_{ac}(H_k) \) has the band structure and hence we can define the \( j \)th band \( \sigma_{kj} = [\lambda_{k,j-1}^+, \lambda_{k,j}^-] \) and the \( j \)th spectral gap \( \gamma_{kj} = (\lambda_{k,j}^+, \lambda_{k,j}^-) \) for each \( j \in \mathbb{N} \). For \( k \in \{1, 2, \cdots, \ell - 1\} \), we have \( \lambda_{k,2j-1}^- \neq \lambda_{k,2j}^+ \) for every \( j \in \mathbb{N} \). For \( k \in \{0, 1, 2, \cdots, \ell - 1\} \setminus \{\frac{N}{2}\} \), we have \( \lambda_{k,2j-1}^- \neq \lambda_{k,2j-1}^+ \) for every \( j \in \mathbb{N} \). Namely, if \( k \in \{0, 1, 2, \cdots, \ell - 1\} \setminus \{\frac{N}{2}\} \), then every spectral gap of \( H_k \) is not degenerate, i.e., \( \gamma_{kj} \neq \emptyset \) is valid for all \( j \in \mathbb{N} \).

Moreover, we obtain the asymptotic behavior of the band edges. For the next theorem, we prepare notations. First, we put

\[
q_n = \int_0^1 q(x) e^{2\pi i x} \, dx, \quad q_{cj,n} = \int_0^1 (1 - 2t)^j q(t) \cos 2n\pi t \, dt, \quad q_{sj,n} = \int_0^1 (1 - 2t)^j q(t) \sin 2n\pi t \, dt
\]

for \( q \in L^2(0,1), j \in \mathbb{N} \) and \( n \in \mathbb{N} \). Furthermore, we designate \( u_{0,12n}^+ = 2n\pi, u_{0,12n+2}^\pm = \frac{2}{3} + 2n\pi, u_{0,12n+4}^\pm = \frac{5}{2} + 2n\pi, u_{0,12n+6}^\pm = \frac{7}{4} + 2n\pi, u_{0,12n+8}^\pm = \frac{5}{3} + 2n\pi, u_{0,12n+10}^\pm = \frac{5}{4} + 2n\pi, u_{0,12n+12}^- = \frac{3}{2} + 2n\pi, u_{0,12n+14}^\pm = \frac{3}{4} + 2n\pi, u_{0,12n+16}^\pm = \frac{5}{6} + 2n\pi, u_{0,12n+18}^\pm = \frac{5}{8} + 2n\pi, u_{0,12n+20}^\pm = \frac{7}{8} + 2n\pi, u_{0,12n+22}^\pm = \frac{3}{5} + 2n\pi, u_{0,12n+24}^\pm = \frac{7}{10} + 2n\pi, u_{0,12n+26}^\pm = \frac{5}{7} + 2n\pi, u_{0,12n+28}^\pm = \frac{3}{8} + 2n\pi, u_{0,12n+30}^\pm = \frac{11}{12} + 2n\pi \) and \( \lambda_{0,12n}^- = \frac{1}{2} + 2n\pi \) for every \( n \in \mathbb{N} \). We also need the notation

\[
q_{s, j, n, p} = \int_0^1 (1 - 2t)^j q(t) \sin u_{\frac{1}{p} + 12n}^\pm (1 - 2t) \, dt
\]

for \( j, n \in \mathbb{N} \) and \( p = 1, 3, 5, 7, 9, 11 \). Then, we have the following results for \( k = 1, 2, \cdots, \ell - 1 \).

**Theorem 1.3.** (i) On the asymptotics for edges of even-numbered spectral gaps, we have the followings:

(a) Let \( k = 1, 2, \cdots, \ell - 1 \). Then, for \( p = 1, 2, 3, 4, 5, 6 \), we have

\[
\lambda_{k,12n+2p}^\pm = (u_{k,12n+2p}^\pm)^2 + q_0 + O\left(\frac{1}{n}\right) \quad \text{as} \quad n \to \infty.
\]  

(1.3)

(b) Let \( k = 0 \). Then, we have the followings:

\[
\lambda_{0,12n+p}^\pm = (u_{0,12n+p}^\pm)^2 + q_0 + O\left(\frac{1}{n}\right) \quad \text{as} \quad n \to \infty \quad \text{for} \quad p = 2, 4, 8, 10,
\]

(1.4)

\[
\lambda_{0,12n+12}^\pm = 4(n+1)^2\pi^2 + q_0 \pm \sqrt{|q_{2n+2}^2| - \frac{8}{27} q_{5,0,2n+2}^2 + O\left(\frac{1}{n}\right)} + O\left(\frac{1}{n}\right) \quad \text{as} \quad n \to \infty.
\]  

(1.5)

\[
\lambda_{0,12n+6}^\pm = (2n+1)^2\pi^2 + q_0 \pm \sqrt{|q_{2n+1}^2| - \frac{8}{27} q_{5,0,2n+1}^2 + O\left(\frac{1}{n}\right)} + O\left(\frac{1}{n}\right) \quad \text{as} \quad n \to \infty.
\]

(1.6)
(ii) On the asymptotics for edges of odd-numbered spectral gaps, we have the followings:
(a) Let \( k \neq \frac{n}{2} \) or \( q \) be even. Then, for \( p = 1, 3, 5, 7, 9, 11 \), we have
\[
\lambda_{k,12n+p}^\pm = (u_{k,12n+p}^\pm)^2 + q_0 + o\left(\frac{1}{n}\right) \quad \text{as } n \to \infty.
\]
(1.7)

(b) Let \( k = \frac{n}{2} \) and \( q \) be not even. Then, we have the followings:
\[
\lambda_{k,12n+p}^\pm = (u_{k,12n+p}^\pm)^2 + q_0 \pm \sqrt{\frac{789}{108}} \sqrt{q_{5,0,n,p}^2 + o\left(\frac{1}{n}\right)} + o\left(\frac{1}{n}\right) \quad \text{if } p = 3, 9 \text{ as } n \to \infty,
\]
(1.8)
\[
\lambda_{k,12n+p}^\pm = (u_{k,12n+p}^\pm)^2 + q_0 \pm \frac{411}{1944} \sqrt{q_{5,0,n,p}^2 + o\left(\frac{1}{n}\right)} + o\left(\frac{1}{n}\right) \quad \text{if } p = 1, 5, 7, 11 \text{ as } n \to \infty.
\]
(1.9)

Furthermore, we obtain the results for the absence of spectral gaps.

**Theorem 1.4.** Let \( q \in L^2(0,1) \) be real-valued. For each \( n \in \mathbb{N} \), we have the followings:

(i) We have \( \gamma_{0,12n-10} = \gamma_{0,12n-8} = \gamma_{0,12n-4} = \gamma_{0,12n-2} = \emptyset \).

(ii) If \( \frac{n}{2} \in \mathbb{N} \) and \( q \) is even, then we have \( \gamma_{\frac{n}{2},12n-(2p-1)} = \emptyset \) for \( p = 1, 2, 3, 4, 5, 6 \).

**Remark 1.1.** In the sense of Lemma 4.5(ii), the evenness of \( q \) in the assumption (ii) is essential. Namely, if \( q \) is not even function, we see the existence of infinitely many present spectral gaps. Especially, there is some \( n_0 \in \mathbb{N} \) such that \( \gamma_{0,12n-1}, \gamma_{0,12n-5}, \gamma_{0,12n-7}, \gamma_{0,12n-11} \neq \emptyset \) for any \( n \geq n_0 \).

Spectral analysis for single-wall carbon nanotubes has been seen in [9, 10, 12]. In [12], spectra for all classes of carbon nanotubes, namely, zigzag, armchair and chiral are taken into account. Korotyaev and Lobanov [10] dealt with the single-wall zigzag carbon nanotubes (See the left one in Fig. 2) and gave the spectral theory including the existence of band structure, the asymptotics of absolutely continuous spectrum and the inverse spectral problems. In order to compare the result in [10] and ours, we quote the former one. For \( \omega \in \hat{Z} := \mathbb{Z} \times f \times \mathbb{Z}_N \), we put \( \hat{f}_\omega = \{ x = \tilde{f}_\omega + i\tilde{e}_\omega \mid 0 \leq t \leq 1 \} \simeq [0,1] \), where \( \tilde{f} = \{ 0, 1, 2 \} \),

\[
\tilde{e}_{n,0,k} = (0,0,1), \quad \tilde{e}_{n,1,k} = \kappa_{n+2k+1} - \kappa_{n+2k} + \frac{\tilde{e}_0}{2}, \quad \tilde{e}_{n,2,k} = \kappa_{n+2k+2} - \kappa_{n+2k+1} - \frac{\tilde{e}_0}{2},
\]
\[
\tilde{r}_{n,0,k} = \kappa_{n+2k} + \frac{3n}{2} \tilde{e}_0, \quad \tilde{r}_{n,1,k} = \tilde{r}_{n,0,k} + \tilde{e}_0, \quad \tilde{r}_{n,2,k} = \tilde{r}_{n+1,0,k}.
\]

Then, the picture of the set \( \hat{f}^N = \bigcup_{\omega \in \hat{Z}} \hat{f}_\omega \) appears in the left side in Fig. 2. Korotyaev and Lobanov assumed that \( N = 2m+1 \) for a fixed \( m \geq 0 \) and investigated the spectrum of the following periodic Schrödinger operator with \( q \in L^2(0,1) \) in \( L^2(\hat{f}^N) = \bigoplus_{\omega \in \hat{Z}} L^2(\Gamma_\omega) \):

\[
(\hat{H}f_\omega)(x) = -f''_\omega(x) + q(x)f_\omega(x), \quad x \in (0,1) \simeq \Gamma_\omega, \quad \omega \in \hat{Z},
\]
As shown in [10, Theorem 1.1], the authors gave the unitarily equivalence between the operator $\tilde{H}$ and $\bigoplus_{k=1}^{N} \tilde{H}_k$, where $\tilde{H}_k$ is the following operator in $L^2(\Gamma^1)$ for $k=1,2,\cdots,N$:

$$(\tilde{H}_kf_{n,j})(x) = -f''_{n,j}(x) + q(x)f_{n,j}(x), \quad x \in (0,1) \ni \Gamma_{n,j}^0 := \Gamma_{n,j,1}^0, \quad (n,j) \in \tilde{Z}_1 := Z \times J.$$ 

As shown in [10, Theorem 1.1], the authors gave the unitarily equivalence between the operator $\tilde{H}$ and $\bigoplus_{k=1}^{N} \tilde{H}_k$, where $\tilde{H}_k$ is the following operator in $L^2(\Gamma^1)$ for $k=1,2,\cdots,N$:

$$\text{Dom}(\tilde{H}) = \left\{ \bigoplus_{\omega \in Z} f_\omega \in L^2(\Gamma^N), \begin{array}{l} \bigoplus_{\omega \in Z} (-f''_\omega + qf_\omega) \in L^2(\Gamma^N), \\ -f'_{n,0,k}(1) + f'_{n,1,k}(0) - f'_{n,2,k-1}(1) = 0, \\ f_{n,1,k}(0) = f_{n,0,k}(1) = f_{n,2,k-1}(1), \\ f''_{n,0,k}(0) - f''_{n,1,k}(1) + f''_{n,2,k}(0) = 0, \\ f_{n,1,k}(1) = f_{n+1,0,k}(0) = f_{n+2,k}(0) \end{array} \right\} \cup \sigma_{\infty}(\tilde{H}_k) \cup \sigma_{\infty}(\tilde{H}_k).$$

Here, we recall that $s = e^{2\pi i N}$. The picture of the degenerate zigzag nanotube is in Fig. 5.

According to [10, Theorem 1.3], the spectrum of $\tilde{H}_k$ consists of the absolutely continuous spectrum and the flat bands, namely, the set of eigenvalues with infinite multiplicities: $\sigma(\tilde{H}_k) = \sigma_{ac}(\tilde{H}_k) \cup \sigma_{\infty}(\tilde{H}_k)$. Moreover, they proved that $\sigma_{\infty}(\tilde{H}_k) = \sigma_D(L)$. Especially, every eigenvalue with infinite multiplicities of $H_k$ is in the closure of the spectral gaps of $L := -\frac{d^2}{dx^2} + q(x)$ in a wide sense, that is, $\bigcup_{j=1}^{n} [\lambda_{2j-1}, \lambda_{2j}]$. In the case of supergraphene-based zigzag carbon nanotubes, there are more eigenvalues with the infinite multiplicities in comparison with this result (see Theorem 1.1). In particular, we see that additional eigenvalues appear in the spectral band $\bigcup_{j=1}^{n} [\lambda_{2j-2}, \lambda_{2j-1}]$. Besides, Lemma 3.2 (i) and (iv) below implies that all eigenvalues of $H_k$ appears in the closure of even-numbered spectral gaps $[\lambda_{k,2}, \lambda_{k,2}]$ in a wide sense of $H_k$ for each $k=0,1,2,\cdots,\ell-1$. In the even case, namely, $N=2\ell$ and $\ell \in \mathbb{N}$, Theorem 1.1 (ii) implies that the absolutely continuous spectrum of $H_{N/2}$ does not exist. In this case, $\sigma(\tilde{H}_{N/2})$ only consists of the eigenvalues with
the infinite multiplicities. Examples of the spectra without the band structure for periodic Schrödinger operators can be seen in [9, 17]. Although those examples are seen in a magnetic field, there is no magnetic field in our case. As seen in Theorem 1.4, there are infinitely many absent spectral gaps regardless of (even) potentials and the infinitely many bands merge. This might happen due to the carbine-like chain of supergraphene-based carbon nanotubes. The strength of the carbine-like chains of supergraphene-based carbon nanotubes, namely, the strength of the structure, can be stronger than the strength of the potentials. As a future work, we might be interested in the spectral properties in the case where there are more carbons on the edges of hexagons and so on.

We give the plan of this paper. In Section 2, we prove Theorem 1.1. Namely, we make a discriminant of \( H_k \) and give eigenfunctions supported on a compact set for each eigenvalues with infinite multiplicities. In Section 3, we analyze the discriminant of \( H_k \) and show the existence of the band structure of \( H_k \). Finally, we shall give the asymptotics of the band edges of the spectrum of \( H_k \) in the last section. In Section 4, we also obtain the absence of the spectral gaps stated in Theorem 1.4.

## 2 Proof of Theorem 1.1

We abbreviate \( \theta(1, \lambda), \theta'(1, \lambda), \varphi(1, \lambda) \) and \( \varphi'(1, \lambda) \) to \( \theta_1, \theta_1', \varphi_1 \) and \( \varphi_1' \) below. In this section, we give the proof of Theorem 1.1. First, we shall show the followings:

**Lemma 2.1.** For a fixed \( N \in \mathbb{N} \), we have \( \sigma_{1/2}(L) \cup \sigma_{-1/2}(L) \subset \sigma_\infty(H_k) \) for \( k = 1, 2, \ldots, N \).

**Proof.** (I) We first show \( \sigma_{1/2}(L) \subset \sigma_\infty(H_k) \). Pick a \( \lambda \in \sigma_{1/2}(L) \), arbitrarily. We put \( v_1(x, \lambda) = \varphi_1\theta(x, \lambda) + \varphi_1'\varphi(x, \lambda) \) and \( v_2(x, \lambda) = \varphi_1\theta(x, \lambda) - \theta_1\varphi(x, \lambda) \).

(a) Assume that \( k = 0 \). Then, we define

\[
\begin{align*}
    u_{0,4}^{(0)}(x, \lambda) &= \varphi(x, \lambda), \quad u_{0,5}^{(0)}(x, \lambda) = v_1(x, \lambda), \quad u_{0,6}^{(0)}(x, \lambda) = v_2(x, \lambda), \\
    u_{0,7}^{(0)}(x, \lambda) &= -\varphi(x, \lambda), \quad u_{0,8}^{(0)}(x, \lambda) = -v_1(x, \lambda), \quad u_{0,9}^{(0)}(x, \lambda) = -v_2(x, \lambda)
\end{align*}
\]

and \( u_{n,i}^{(0)}(x, \lambda) = 0 \) for \( (n, i) \neq (0, 4), (0, 5), (0, 6), (0, 7), (0, 8), (0, 9) \). Furthermore, we define \( u^{(n)} = \{u_{m-n, i}^{(0)}\}_{(m, i) \in \mathbb{Z}} \). Then, we can directly check \( \{u^{(n)}\}_{n \in \mathbb{Z}} \subset \text{Dom}(H_0) \) (especially \( u^{(n)} \) satisfies the boundary Kirchhoff vertex conditions appearing in the domain of \( H_0 \)) and \( H_0u^{(n)} = \lambda u^{(n)} \) for any \( n \in \mathbb{Z} \) by using \( \theta(1, \lambda) + \varphi'(1, \lambda) = 1 \), which is due to \( \lambda \in \sigma_{1/2}(L) \). Thus, we see that \( \lambda \in \sigma_\infty(H_0) \). Hence, we have \( \sigma_{1/2}(L) \subset \sigma_\infty(H_0) \).

(b) Assume that \( k = 1, 2, \ldots, N-1 \). Then, we put \( \alpha_k = -1 + s^{-k}, \beta_k = \frac{1-s^{-k}}{1-s}, \gamma_k = -\frac{1-s^{-k}}{1-s} \),

\[
\begin{align*}
    u_{0,4}^{(0)}(x, \lambda) &= \varphi(x, \lambda), \quad u_{0,5}^{(0)}(x, \lambda) = v_1(x, \lambda), \quad u_{0,6}^{(0)}(x, \lambda) = v_2(x, \lambda), \\
    u_{0,7}^{(0)}(x, \lambda) &= -s^{-k}\varphi(x, \lambda), \quad u_{0,8}^{(0)}(x, \lambda) = -s^{-k}v_1(x, \lambda), \quad u_{0,9}^{(0)}(x, \lambda) = -s^{-k}v_2(x, \lambda),
\end{align*}
\]
If \( n \neq 1 \) or \( (n,j) \neq (0,4),(0,5),(0,6) \) is valid, then we define \( u^{(0)}_{n,j}(x,\lambda) = 0 \). Then, for any \( n \in \mathbb{Z} \), we see that \( u^{(n)} := \{ u^{(0)}_{m-n,j} \}_{(m,j) \in \mathbb{Z}} \) is an eigenvalue of \( H_k \). So, we obtain \( \sigma_{1/2}(L) \subset \sigma_{\infty}(H_k) \).

(II) Next, we show \( \sigma_{-1/2}(L) \subset \sigma_{\infty}(H_k) \). Pick a \( \lambda \in \sigma_{-1/2}(L) \), arbitrarily. Note that

\[
\theta(1,\lambda) + \varphi^\prime(1,\lambda) = -1
\]

for this \( \lambda \). Let us give infinitely many eigenvalues of \( H_0 \) for \( \lambda \).

(a) Assume that \( k = 0 \). Then, we define

\[
\begin{align*}
u^{(0)}_{0,4}(x,\lambda) &= \varphi(x,\lambda), &
u^{(0)}_{0,5}(x,\lambda) &= v_1(x,\lambda), &
u^{(0)}_{0,6}(x,\lambda) &= -v_2(x,\lambda), \\
u^{(0)}_{0,7}(x,\lambda) &= -\varphi(x,\lambda), &
u^{(0)}_{0,8}(x,\lambda) &= -v_1(x,\lambda), &
u^{(0)}_{0,9}(x,\lambda) &= v_2(x,\lambda)
\end{align*}
\]

and \( u^{(0)}_{n,j}(x,\lambda) = 0 \) for \( (n,j) \neq (0,4),(0,5),(0,6),(0,7),(0,8),(0,9) \). For \( n \in \mathbb{Z} \), we put

\[
\begin{align*}u^{(n)} &= \{ u^{(0)}_{m-n,j} \}_{(m,j) \in \mathbb{Z}}.
\end{align*}
\]

(b) Assume that \( k = 1,2,\cdots,N-1 \). Then, we define

\[
\begin{align*}
u^{(0)}_{0,4}(x,\lambda) &= \varphi(x,\lambda), &
u^{(0)}_{0,5}(x,\lambda) &= v_1(x,\lambda), &
u^{(0)}_{0,6}(x,\lambda) &= -v_2(x,\lambda), \\
u^{(0)}_{0,7}(x,\lambda) &= -s^{-k}\varphi(x,\lambda), &
u^{(0)}_{0,8}(x,\lambda) &= -s^{-k}v_1(x,\lambda), &
u^{(0)}_{0,9}(x,\lambda) &= s^{-k}v_2(x,\lambda), \\
u^{(0)}_{1,1}(x,\lambda) &= -\alpha_k\varphi(x,\lambda), &
u^{(0)}_{1,2}(x,\lambda) &= -\alpha_kv_1(x,\lambda), &
u^{(0)}_{1,3}(x,\lambda) &= \alpha_kv_2(x,\lambda), \\
u^{(0)}_{1,4}(x,\lambda) &= \beta_k\varphi(x,\lambda), &
u^{(0)}_{1,5}(x,\lambda) &= \beta_kv_1(x,\lambda), &
u^{(0)}_{1,6}(x,\lambda) &= -\beta_kv_2(x,\lambda), \\
u^{(0)}_{1,7}(x,\lambda) &= \gamma_k\varphi(x,\lambda), &
u^{(0)}_{1,8}(x,\lambda) &= \gamma_kv_1(x,\lambda), &
u^{(0)}_{1,9}(x,\lambda) &= -\gamma_kv_2(x,\lambda).
\end{align*}
\]

If \( n \neq 1 \) or \( (n,j) \neq (0,4),(0,5),(0,6) \) is valid, then we define \( u^{(0)}_{n,j}(x,\lambda) = 0 \). For \( n \in \mathbb{Z} \), we put

\[
\begin{align*}u^{(n)} &= \{ u^{(0)}_{m-n,j} \}_{(m,j) \in \mathbb{Z}}.
\end{align*}
\]

**Lemma 2.2.** For a fixed \( N \in \mathbb{N} \), we have \( \sigma_k(D) \subset \sigma_{\infty}(H_k) \) for \( k = 1,2,\cdots,N \).

**Proof.** Pick a \( \lambda \in \sigma_k(D) \). Let us give infinitely many eigenfunctions for this \( \lambda \). We put

\[
\eta = 1 - e^s \zeta,
\]

where \( \zeta = \varphi^\prime(1,\lambda) \) and \( s = \frac{i2\pi}{N} \).

Assume that \( \eta = 0 \). Then, we define

\[
\begin{align*}
u^{(0)}_{0,4}(x,\lambda) &= \varphi(x,\lambda), &
u^{(0)}_{0,5}(x,\lambda) &= c\varphi(x,\lambda), &
u^{(0)}_{0,6}(x,\lambda) &= c^2\varphi(x,\lambda), \\
u^{(0)}_{0,7}(x,\lambda) &= c^5 \varphi(1-x,\lambda), &
u^{(0)}_{0,8}(x,\lambda) &= c^4 \varphi(1-x,\lambda), &
u^{(0)}_{0,9}(x,\lambda) &= c^3 \varphi(1-x,\lambda)
\end{align*}
\]

and \( u^{(0)}_{n,j}(x,\lambda) = 0 \) for \( (n,j) \neq (0,4),(0,5),(0,6),(0,7),(0,8),(0,9) \). For any \( n \in \mathbb{Z} \), we define \( u^{(n)} = \{ u^{(0)}_{m-n} \} \). Then, we see that \( u^{(n)} \in \text{Dom}(H_k) \) and solves \( H_k u^{(n)} = \lambda u^{(n)} \). Thus, we obtain infinitely many eigenfunctions \( \{ u^{(n)} \}_{n \in \mathbb{Z}} \).
Assume that $\eta \neq 0$. Then, we define

\[
\begin{align*}
  u_{-1,4}^{(0)}(x, \lambda) &= s^k c^3 \varphi(x, \lambda), \\
  u_{-1,5}^{(0)}(x, \lambda) &= s^k c^4 \varphi(x, \lambda), \\
  u_{-1,6}^{(0)}(x, \lambda) &= s^k c^5 \varphi(x, \lambda), \\
  u_{0,1}^{(0)}(x, \lambda) &= \eta \varphi(x, \lambda), \\
  u_{0,2}^{(0)}(x, \lambda) &= c\eta \varphi(x, \lambda), \\
  u_{0,3}^{(0)}(x, \lambda) &= c^2 \eta \varphi(x, \lambda), \\
  u_{0,4}^{(0)}(x, \lambda) &= c^3 \varphi(x, \lambda), \\
  u_{0,5}^{(0)}(x, \lambda) &= c^4 \varphi(x, \lambda), \\
  u_{0,6}^{(0)}(x, \lambda) &= c^5 \varphi(x, \lambda), \\
  u_{0,7}^{(0)}(x, \lambda) &= c^6 \varphi(x, \lambda), \\
  u_{0,8}^{(0)}(x, \lambda) &= c^7 \varphi(x, \lambda), \\
  u_{0,9}^{(0)}(x, \lambda) &= c^8 \varphi(x, \lambda),
\end{align*}
\]

and $u_{n,j}^{(0)} = 0$ for $n \neq 1$ or $(n,j) \not= (-1,4), (-1,5), (-1,6), (-1,7), (-1,8), (-1,9)$. Putting $u^{(n)} = \{u_{n,j}^{(0)}\}$ for any $n \in \mathbb{Z}$, we see that $u^{(n)}$ is an eigenfunction for each $n \in \mathbb{Z}$. Thus, we obtain infinitely many eigenfunctions $\{u^{(n)}\}_{n \in \mathbb{Z}}$.

**Proof of Theorem 1.1.** We next examine the set $\sigma(H_k) \setminus (\sigma_{1/2}(L) \cup \sigma_{-1/2}(L) \cup \sigma_D(L))$. In order to examine this set, we utilize a direct integral decomposition for $H_k$ (see [6, 19]). For $\mu \in [0, 2\pi)$, we define the Hilbert space $\mathcal{H}_{\mu} = \mathcal{H} \otimes_{j=1}^{\infty} L^2(\Gamma, d\mu)$. Considering the Hilbert space

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

and the unitary operator $U : L^2(\Gamma) \rightarrow \mathcal{H}$ defined as

\[
(Uf)(x, \mu) = \sum_{p \in \mathbb{Z}} e^{ip\mu} f(x-p), \quad f = (f_n(x))_{n \in \mathbb{Z}} = (f_{n,j}(x))_{(n,j) \in \mathbb{Z} \times \mathbb{Z} \in L^2(\Gamma),}
\]

we obtain a direct integral representation of $H_k$ like

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

where $H_k(\mu)$ is a fiber operator in $\mathcal{H}_{\mu}$ defined as

\[
(H_k(\mu)f_j)(x) = -f''_j(x) + q(x)f_j(x), \quad x \in (0, 1) \simeq \mathcal{H}_{\mu}, \quad j \in \mathbb{J},
\]

\[
\text{Dom}(H_k(\mu)) = \left\{ \begin{array}{l}
\bigoplus_{j=1}^{9} (-f''_j + qf_j) \in \mathcal{H}_{\mu}, \\
  f_1(1) = f_2(0), \quad f'_1(1) = f'_2(0), \\
  f_2(1) = f_3(0), \quad f'_2(1) = f'_3(0), \\
  f_3(1) = f_4(0) - s^k f_7(0), \quad -f'_3(1) + f'_4(0) + s^k f'_7(0) = 0, \\
  f_4(1) = f_5(0), \quad f'_4(1) = f'_5(0), \\
  f_5(1) = f_6(0), \quad f'_5(1) = f'_6(0), \\
  f_6(1) = f_7(0), \quad f'_6(1) = f'_7(0), \\
  f_7(1) = f_8(0), \quad f'_7(1) = f'_8(0), \\
  f_8(1) = f_9(0), \quad f'_8(1) = f'_9(0), \\
  f_9(1) = e^{i\mu} f_1(0), \quad -f'_9(1) - f'_1(1) + e^{i\mu} f'_1(0) = 0.
\end{array} \right\}
\]
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 \( H_k(\mu) \), which 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

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

In Lemmas 2.1 and 2.2, we found that \( \sigma_{1/2}(L) \cup \sigma_{-1/2}(L) \cup \sigma_D(L) \subset \sigma_\infty(H_k) \) for \( k = 1,2,\cdots,N \). We below examine the set \( \sigma(H_k) \setminus (\sigma_{1/2}(L) \cup \sigma_{-1/2}(L) \cup \sigma_D(L)) \). We pick \( \lambda \not\in \sigma_{1/2}(L) \cup \sigma_{-1/2}(L) \cup \sigma_D(L) \), arbitrarily. For this \( \lambda \), we consider the characteristic equation \( H_k(\mu)f = \lambda f \) for \( 0 \neq f = (f_j)_{j=1}^6 \in \text{Dom}(H_k(\mu)) \). Namely, we consider the following system:

\[
\begin{align*}
-f''_j(x) + q(x)f_j(x) &= \lambda f_j(x), \quad x \in (0,1) \equiv \Gamma_{0\mu}^0, \quad j \in \mathbb{J}, \quad (2.1) \\
f_1(1) &= f_2(0), \quad f_2(1) = f_3(0), \quad f_4(1) = f_5(0), \quad (2.2) \\
f_5(1) &= f_6(0), \quad f_7(1) = f_8(0), \quad f_8(1) = f_9(0), \quad (2.3) \\
f_9(1) &= f_4(0) = s^j \phi_7(0), \quad f_6(1) = f_9(1) = e^{i\mu} f_1(0), \quad (2.4) \\
f_1'(1) &= f_2'(0), \quad f_2'(1) = f_3'(0), \quad f_4'(1) = f_5'(0), \quad (2.5) \\
f_5'(1) &= f_6'(0), \quad f_7'(1) = f_8'(0), \quad f_8'(1) = f_9'(0), \quad (2.6) \\
-f_3'(1) + f_4'(0) + \sigma \phi_7(0) &= 0, \quad -f_6'(1) - f_9'(1) + e^{i\mu} f_1'(0) = 0. \quad (2.7)
\end{align*}
\]

We first solve (2.1). Since \( \lambda \not\in \sigma_D(L) \), we have \( \varphi_1 = \varphi(1,\lambda) \neq 0 \). Thus, any solution to \(-f'' + qf = \lambda f \) is given as

\[
f(x,\lambda) = \theta(x,\lambda)f(0,\lambda) + \frac{\varphi(x,\lambda)}{\varphi_1}(f(1,\lambda) - \theta_1 f(0,\lambda))
\]

on \([0,1]\) for \( \lambda \not\in \sigma_D(L) \). Let us put \( X_1 = f_1(0) \), \( X_2 = f_2(0) \), \( X_3 = f_3(0) \), \( X_4 = f_4(0) \), \( X_5 = f_5(0) \), \( X_6 = f_6(0) \), \( X_7 = f_7(0) \), \( X_8 = f_8(0) \) and \( w(x,\lambda) = \theta(x,\lambda) - \frac{\theta(1,\lambda)}{\varphi_1(1,\lambda)} \varphi(x,\lambda) \). Then, we have

\[
\begin{align*}
f_1(x,\lambda) &= w(x,\lambda)X_1 + \frac{\varphi(x,\lambda)}{\varphi_1}X_2, \quad f_2(x,\lambda) = w(x,\lambda)X_2 + \frac{\varphi(x,\lambda)}{\varphi_1}X_3, \\
f_3(x,\lambda) &= w(x,\lambda)X_3 + \frac{\varphi(x,\lambda)}{\varphi_1}X_4, \quad f_4(x,\lambda) = w(x,\lambda)X_4 + \frac{\varphi(x,\lambda)}{\varphi_1}X_5, \\
f_5(x,\lambda) &= w(x,\lambda)X_5 + \frac{\varphi(x,\lambda)}{\varphi_1}X_6, \quad f_6(x,\lambda) = w(x,\lambda)X_6 + \frac{\varphi(x,\lambda)}{\varphi_1}e^{i\mu}X_1, \\
f_7(x,\lambda) &= w(x,\lambda)X_7 + \frac{\varphi(x,\lambda)}{\varphi_1}X_8, \quad f_8(x,\lambda) = w(x,\lambda)X_7 + \frac{\varphi(x,\lambda)}{\varphi_1}X_8, \\
f_9(x,\lambda) &= w(x,\lambda)X_8 + \frac{\varphi(x,\lambda)}{\varphi_1}e^{i\mu}X_1.
\end{align*}
\]
due to (2.2), (2.3), (2.4) and (2.8). Substituting these 9 formulas into (2.5), (2.6), (2.7), we obtain a system on \( \{ X_j \}_{j=1}^8 \) as follows:

\[
\begin{align*}
X_1 - 2\Delta X_2 + X_3 &= 0, \\
X_2 - 2\Delta X_3 + X_4 &= 0, \\
X_3 - (2\theta_1 + \varphi_1') X_4 + X_5 + s^k X_7 &= 0, \\
X_4 - 2\Delta X_5 + X_6 &= 0, \\
\varepsilon^{ij} X_1 + X_5 - 2\Delta X_6 &= 0, \\
s^{-k} X_4 - 2\Delta X_7 + X_8 &= 0, \\
\varepsilon^{ij} X_1 + X_7 - 2\Delta X_8 &= 0, \\
- (2\varphi_1' + \theta_1) \varepsilon^{ij} X_1 + \varepsilon^{ij} X_2 + X_6 + X_8 &= 0.
\end{align*}
\]

Here, we recall \( \Delta \) is the discriminant of \( \sigma(L) \): \( \Delta = \frac{\theta_1 + \varphi_1'}{2} \). Let \( M_k(\lambda, \mu) \) be the coefficient matrix of the system on \( X_1, X_2, \ldots, X_8 \):

\[
M_k(\lambda, \mu) = \begin{pmatrix}
1 & -2\Delta & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & -2\Delta & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & -(2\theta_1 + \varphi_1') & 1 & 0 & s^k & 0 \\
0 & 0 & 0 & 1 & -2\Delta & 1 & 0 & 0 \\
\varepsilon^{ij} & 0 & 0 & 0 & 1 & -2\Delta & 0 & 0 \\
0 & 0 & 0 & s^{-k} & 0 & 0 & -2\Delta & 1 \\
- (2\varphi_1' + \theta_1) \varepsilon^{ij} & 0 & 0 & 0 & 0 & 1 & -2\Delta & 1 \\
\varepsilon^{ij} & 0 & 0 & 0 & 1 & 0 & 0 & 1
\end{pmatrix}.
\]

The system has only the trivial solution \( X = (X_1, X_2, \ldots, X_8) = 0 \), which implies that \( f = (f_j)_{j=1}^8 \equiv 0 \), if and only if \( \det M_k(\lambda, \mu) \neq 0 \). So, for each \( \mu \in [0, 2\pi), \lambda \in \mathbb{R} \setminus \sigma_D(L) \) is an eigenvalue of \( H_k(\mu) \) if and only if \( \det M_k(\lambda, \mu) = 0 \). Straightforward calculations yield

\[
e^{-i\mu} \det M_k(\lambda, \mu) = (4\Delta^2 - 1) \left[ (e^{-i\mu} + s^{-k} e^{-i\mu} + s^k e^{i\mu} + e^{i\mu})
- 128\Delta^6 + (208 - 16\theta_1 \varphi_1') \Delta^4 + 8\Delta^2 (\theta_1 \varphi_1' - 10) + 3 + s^k + s^{-k} - \theta_1 \varphi_1' \right]. \tag{2.9}
\]

Using \( s = e^{i\frac{\theta_1}{N}} \) and \( (1 + s^k) e^{i\mu} = \cos \mu + \cos \left( \frac{2\pi k}{N} + \mu \right) + i (\sin \mu + \sin \left( \frac{2\pi k}{N} + \mu \right)) \), we have

\[
e^{-i\mu} + s^{-k} e^{-i\mu} + s^k e^{i\mu} + e^{i\mu} = 2 \left( \cos \mu + \cos \left( \frac{2\pi k}{N} + \mu \right) \right) = 4 \cos \left( \frac{\pi k}{N} + \mu \right) \cos \frac{\pi k}{N}.
\]

This combined with (2.9) and \( \theta_1 \varphi_1' = \Delta^2 - \Delta^- \) means that

\[
e^{-i\mu} \det M_k(\lambda, \mu) = (4\Delta^2 - 1) \left[ 4 \cos \left( \frac{\pi k}{N} + \mu \right) \cos \frac{\pi k}{N}
- 144\Delta^6 + (216 + 16\Delta^-) \Delta^4 - (8\Delta^- + 81) \Delta^2 + 3 + s^k + s^{-k} + \Delta^- \right].
\]
Since $4\Delta^2 - 1 \neq 0$ for $\lambda \notin \sigma_{1/2}(L) \cup \sigma_{-1/2}(L)$, we see that $\det M_k(\lambda, \mu) = 0$ is equivalent to
\begin{equation}
4\cos\left(\frac{\pi k}{N} + \mu\right) \cos\frac{\pi k}{N} = 144\Delta^6 - (216 + 16\Delta^2)\Delta^4 + (8\Delta^2 + 81)\Delta^2 - (3 + s^k + s^{-k} + \Delta^2) \tag{2.10}
\end{equation}
for $\lambda \notin \sigma_{1/2}(L) \cup \sigma_{-1/2}(L) \cup \sigma_D(L)$. This formula is called the dispersion relation, where $\mu$ is the one-dimensional quasimomentum. For each $\mu \in [0, 2\pi)$, we see that $\lambda \in \mathbb{R} \setminus (\sigma_{1/2}(L) \cup \sigma_{-1/2}(L) \cup \sigma_D(L))$ satisfies (2.10) if and only if $\lambda \in \sigma_{\infty}(H_{N/2})$.

Consider the case where $(N,k) \neq (2\ell, \ell)$. Then, we have
\[
\sigma_{ac}(H_k) \setminus (\sigma_{1/2}(L) \cup \sigma_{-1/2}(L) \cup \sigma_D(L)) = \left\{ \lambda \in \mathbb{R} \mid D(k, \lambda) = \cos\left(\frac{\pi k}{N} + \mu\right) \right\} \setminus (\sigma_{1/2}(L) \cup \sigma_{-1/2}(L) \cup \sigma_D(L))
\]
\[
= \left\{ \lambda \in \mathbb{R} \mid D(k, \lambda) \in [-1, 1] \right\} \setminus (\sigma_{1/2}(L) \cup \sigma_{-1/2}(L) \cup \sigma_D(L)).
\]

Since an absolutely continuous spectrum is a closed set, we take the closure of this equation and hence obtain $\sigma_{ac}(H_k) = \{ \lambda \in \mathbb{R} \mid -1 \leq D(k, \lambda) \leq 1 \}$. \qed

### 3. Band structure of $\sigma(H_k)$

In this section, we establish the proof of Theorem 1.2 and make sure the existence of the band structure of $H_k$. Throughout this section, we consider $k = 0, 1, \cdots, \ell - 1$, where $N = 2\ell + 1$ or $N = 2\ell + 2$ for a fixed $\ell \in \mathbb{N}$. In order to grasp the behavior of the discriminant $D(k, \lambda)$, we shall establish lemmas. First, we consider the unperturbed case: $q \equiv 0$. In this case, we see that the discriminant is
\[
D_0(k, \lambda) = \frac{1}{4\cos^2\frac{\pi k}{N}} \left\{ 144\cos^6\sqrt{\lambda} - 216\cos^4\sqrt{\lambda} + 81\cos^2\sqrt{\lambda} - 3 - 3\cos\frac{2\pi k}{N} \right\}.
\]

On the behavior of this function, we obtain the followings (see also Fig. 6):\n
**Lemma 3.1.** Let $\lambda \in \mathbb{R}$.

(i) As long as $\lambda \in (0, \frac{\pi}{6}), (\frac{\pi}{3}, \frac{\pi}{2}), (\frac{3\pi}{2}, \frac{5\pi}{6}), (\pi, \frac{7\pi}{6}), (\frac{4\pi}{3}, \frac{3\pi}{2}), (\frac{5\pi}{3}, \frac{11\pi}{6}) \mod 2\pi$, we see that $D_0(k, \lambda)$ strictly decreases.

(ii) As long as $\lambda \in (\frac{\pi}{6}, \frac{\pi}{3}), (\frac{\pi}{2}, \frac{2\pi}{3}), (\frac{5\pi}{6}, \pi), (\frac{7\pi}{6}, \frac{4\pi}{3}), (\frac{3\pi}{2}, \frac{5\pi}{3}), (\frac{11\pi}{6}, 2\pi) \mod 2\pi$, we see that $D_0(k, \lambda)$ strictly increases.

(iii) As long as $\lambda \in (-\infty, 0)$, we see that $D_0(k, \lambda)$ strictly decreases.
We first deal with Proof. Thus, we see that (i) and (ii) hold true.

Fig. 6: The graph of $D_0(0,\lambda), D_0(1,\lambda), D_0(2,\lambda), D_0(3,\lambda), D_0(4,\lambda), D_0(5,\lambda)$ and $\cos \sqrt{\lambda}$ in the case where $N=15$. This picture hinted the results of Theorem 1.2. Namely, one can numerically expect that $\tilde{\lambda}_{k,2j} = \lambda_{k,2j}^+$ for $k = \frac{N}{2}$ and $\lambda_{k,2j-1}^- = \lambda_{k,2j-1}^-$ for $k = 0$ in the case where $q \equiv 0$.

Proof. We first deal with $\lambda \geq 0$. Putting $x = \cos^2 \sqrt{\lambda} \in [0,1]$, we consider the behavior of $f_k(x) = 144x^3 - 216x^2 + 81x - (3+2\cos \frac{2\pi k}{N})$. By $f_k'(x) = 432x^2 - 432x + 81 = 432(x - \frac{1}{4})(x - \frac{3}{4})$, we see $f_k(x)$ increases (decreases, respectively) if $x \in (0, \frac{1}{4}) \cup (\frac{3}{4}, 1)$ ($x \in (\frac{1}{4}, \frac{3}{4})$, respectively). Thus, we see that (i) and (ii) hold true.

Next, we deal with $\lambda < 0$. Since $f_k'(x) > 0$ for $x = \cosh^2 \sqrt{-\lambda} \in (1, \infty)$, we have (iii). \(\square\)

Getting a hint from this lemma, we obtain the first properties for $D(k,\lambda)$. In order to prove the following lemma, we prepare the formula

$$D(k,\lambda) = \tilde{D}_0(k,\lambda) - \frac{\Delta^2(\lambda)}{4\cos \frac{2\pi k}{N}} (4\Delta^2 - 1)^2,$$

where

$$\tilde{D}_0(k,\lambda) = \frac{1}{4\cos \frac{2\pi k}{N}} \left\{ 144\Delta^6(\lambda) - 216\Delta^4(\lambda) + 81\Delta^2(\lambda) - \left( 3 + 2\cos \frac{2\pi k}{N} \right) \right\}.$$

**Lemma 3.2.** For $k = 0,1,2,\cdots, \ell - 1$, we have the followings:

(i) If $\Delta^2 = \frac{1}{4}$, then we have $D(k,\lambda) \geq 1$.

(ii) If $\Delta^2 = \frac{3}{4}$, then we have $D(k,\lambda) \leq -1$.

(iii) If $\Delta = 0$, then we have $D(k,\lambda) \leq -1$.

(iv) If $\lambda \in \sigma_D(L)$, then we have $D(k,\lambda) \geq 1$.

Proof. (i) Note that $\cos \frac{\pi k}{N} \in (0,1]$ for $k = 0,1,\cdots, \ell - 1$. It follows by $\Delta^2 = \frac{1}{4}$ that $D(k,\lambda) = \frac{6 - 2\cos \frac{2\pi k}{N}}{4\cos \frac{2\pi k}{N}} = \frac{3}{2} - \cos \frac{2\pi k}{N}$. Putting $g(c) = \frac{3}{2} - c$ for $c \in (-1,1]$, we have $g'(c) = -\frac{1}{2} - 1 < 0$. Hence, $g$ strictly decreases and $g(c) \geq g(1) = 1$ for $c \in (0,1]$. Thus, we obtain $D(k,\lambda) \geq 1$. 

(ii) It follows by \( \Delta^2 = \frac{3}{4} \) that \( D(k, \lambda) = -\frac{1+4\cos^2 \frac{\pi k}{N}}{4\cos \frac{\pi}{N}} - \frac{\Delta^2}{4\cos \frac{\pi}{N}} \). The inequality of arithmetic and geometric means yields \( 1+4c^2 \geq 1 \) for \( c \in (0,1] \). This is why we obtain \( D(k, \lambda) \leq -1 \).

(iii) It follows by \( \Delta = 0 \) that \( D(k, \lambda) = -\frac{3+2\cos \frac{\pi}{N}}{4\cos \frac{\pi}{N}} - \frac{\Delta^2}{4\cos \frac{\pi}{N}} = -\frac{4\cos^2 \frac{\pi}{N} + 1}{4\cos \frac{\pi}{N}} - \frac{\Delta^2}{4\cos \frac{\pi}{N}} \leq -1 \).

(iv) It follows by \( \lambda \in \sigma_D(L) \) that \( q_1 = 0 \) and hence \( 1 = \theta_1 q'_1 \). This combined with \( \Delta^2 - \Delta^2 = \theta_1 q'_1 \) yields \( -\Delta^2 = 1 - \Delta^2 \). Substituting this into (3.1), we have

\[
4\cos \frac{\pi k}{N} D(k, \lambda) = 128\Delta^6 - 192\Delta^4 + 72\Delta^2 - 2 \left( 1 + \cos \frac{2\pi k}{N} \right).
\]

Putting \( g(x) = 128x^3 - 192x^2 + 72x - 2 \left( 1 + \cos \frac{2\pi k}{N} \right) \), we have \( g'(x) = 384 \left( x - \frac{1}{2} \right)^2 - 24 \). Since \( \Delta^2 \geq 1 \) for \( \lambda \in \sigma_D(L) \), we consider \( x \geq 1 \). For \( x \geq 1 \), we have \( g'(x) \geq g'(1) = 72 > 0 \). Thus, we have \( g(x) \geq g(1) \) for \( x \geq 1 \). This implies that

\[
4\cos \frac{\pi k}{N} D(k, \lambda) \geq g(1) = 128 - 192 + 72 - 2 \left( 1 + \cos \frac{2\pi k}{N} \right) = 6 - 2\cos \frac{2\pi k}{N}.
\]

In the same way as proof of (i), we obtain \( D(k, \lambda) \geq 1 \).

**Remark 3.1.** From the proof of Lemma 3.2, we see the followings:

- In the statements of Lemma (i) and (iv), we have \( D(k, \lambda) > 1 \) for \( k = 1, 2, \ldots, \ell - 1 \).
- In the statements of Lemma (ii) and (iii), we have \( D(k, \lambda) < -1 \) for \( k \in \{ 0, 1, 2, \ldots, \ell - 1 \} \setminus \{ \frac{N}{3} \} \).

Let \( c \in [-1,1] \). Although \( D_0(k, \lambda) = c \) is an equation with the degree 6 on \( \cos \sqrt{\lambda} \), it is also a cubic equation on \( \cos^2 \sqrt{\lambda} \). It is well-known for any cubic equation that there is the formula for its algebraic solutions by Cardano. However, since it needs a non-real cubic root of 1, it is complicated. To find the solution to \( D_0(k, \lambda) = c \), we utilize the method established by François Viète in the 16th century to give analytic solutions of the limited cubic equations such that every solution is real. For constants \( p < 0 \) and \( q \in \mathbb{R} \) and a cubic equation \( z^3 + pz + q = 0 \), let us recall that the discriminant of the cubic equation is \( D = -(4p^3 + 27q^2) \). If \( D > 0 \), then the corresponding cubic equation has different three real solutions. In the case where \( D > 0 \), Viète showed that the three real roots of \( z^3 + pz + q = 0 \) are given by

\[
a_k = 2\sqrt{-\frac{p}{3}} \cos \left( \frac{1}{3} \arccos \left( \frac{3q}{2p} \sqrt{-\frac{3}{p}} \right) - \frac{2\pi k}{3} \right), \quad k = 0, 1, 2.
\]

**Lemma 3.3.** (i) Let \( (c,k) \neq (1,0), (-1, \frac{N}{3}) \). Then, the solutions to \( D_0(\lambda) = c \) on \( \cos \sqrt{\lambda} \) are \( \cos \sqrt{\lambda} = \frac{A_0(c,k)}{A_1(c,k)}, A_1(c,k), A_2(c,k) \), where

\[
A_m(c,k) = \frac{1}{2} \cos \left( \theta_k(c) - \frac{2\pi m}{3} \right) + \frac{1}{2}, \quad m = 0, 1, 2,
\]
Moreover, we see that

\[ \lambda = \cos \frac{2\pi k}{N} < -\frac{1}{2}, \]

whose multiplicity is 2.

Proof. Let \( c \in [-1,1] \). Note that \( D(k,\lambda) = c \) is equivalent to

\[
\cos^2 \sqrt{\lambda} = \frac{3}{2} \cos^4 \sqrt{\lambda} + \frac{9}{16} \cos^2 \sqrt{\lambda} - \frac{1}{144} \left( 3 + 2 \cos \frac{2\pi k}{N} + 4 \cos \frac{\pi k}{N} \right) = 0.
\]

Putting \( \cos^2 \sqrt{\lambda} = z + \frac{1}{2} \), this is moreover equivalent to

\[
z^3 - \frac{3}{16} z - \frac{1}{288} \left( 8 \left( c + \frac{c}{2} \right)^2 - 7 - 2c^2 \right) = 0. \tag{3.2}
\]

(i) Let \((c,k) \neq (1,0), (-1,\frac{N}{k})\). Putting the discriminant for (3.2) is \( D \), we have

\[-12 \times 16^2 D = -81 + \left( 8 \left( c + \frac{c}{2} \right)^2 - 7 - 2c^2 \right)^2 = -81 + f_k^2(c).\]

We claim that \( D > 0 \). To prove this, we shall show that \(-9 < f_k^2(c) < 9 \). Since \( f_k^2(c) \) increases in \( c \in [-1,1] \), we obtain \(-9 \leq 8(c_k - \frac{1}{2})^2 - 9 = g_k^2(-1) \leq g_k^2(1) = 8(c_k + \frac{1}{2})^2 - 9 < 9 \). Moreover, we see that \( g_k^2(c) = 9 \) if and only if \((c,k) = (1,0), (c,k) = (-1,\frac{N}{k})\). Thus, we have \( D > 0 \) and hence (3.2) has different three real solutions. It turns out by the Viète’s formula that the solutions to (3.2) are given by \( \{ a_m \}_{m=0,1,2} \), where \( a_m = \frac{1}{4} \cos \left( \theta_k(c) - \frac{2\pi m}{3} \right) \). Since \( \cos^2 \sqrt{\lambda} = z + \frac{1}{2} \), we have \( \cos^2 \sqrt{\lambda} = A_0(c,k), A_1(c,k), A_2(c,k) \). Thus, we obtain (i).

(ii) Let \((c,k) = (1,0) \). Then, \( D(0,\lambda) = 1 \) is equivalent to \( z^3 - \frac{3}{16} z - \frac{1}{32} = 0 \). By virtue of the factorization \( z^3 - \frac{3}{16} z - \frac{1}{32} = \left( z - \frac{1}{4} \right)^2 \) and \( \cos^2 \sqrt{\lambda} = z + \frac{1}{2} \) implies that \( \cos^2 \sqrt{\lambda} = 1, \frac{1}{2} \).

(iii) Let \((c,k) = (-1,\frac{N}{k}) \). Then, \( D(\frac{N}{k},\lambda) = -1 \) is equivalent to \( z^3 - \frac{3}{16} z + \frac{1}{32} = 0 \). By virtue of the factorization \( z^3 - \frac{3}{16} z + \frac{1}{32} = \left( z - \frac{1}{4} \right)^2 \) implies that \( \cos^2 \sqrt{\lambda} = 0, \frac{1}{4} \).

Although we classified \((c,k)\) into 3 cases for the proof in Lemma 3.3, we can summarize passages as follows due to \( \theta_k(1) = 0 \) and \( \theta_k(-1) = \frac{\pi}{2} \):

**Remark 3.2.** For any \( c \in [-1,1] \) and \( k = 0,1,2,\ldots,\ell - 1 \), the solutions to \( D_0(\lambda) = c \) on \( \cos^2 \sqrt{\lambda} \) are \( \cos \sqrt{\lambda} = \sqrt{A_0(c,k)}, -\sqrt{A_0(c,k)}, \sqrt{A_1(c,k)}, -\sqrt{A_1(c,k)}, \sqrt{A_2(c,k)}, -\sqrt{A_2(c,k)} \), where \( A_0(c,k), A_1(c,k), A_2(c,k) \) are the ones stated in Lemma 3.3. Moreover, for a fixed \( k = 0,1,2,\ldots,\ell - 1 \), we see that \( \theta_k(c) \in [0,\frac{\pi}{2}] \) increases in \( c \in [-1,1] \) since \( f_k^2(c) \in [-9,9] \) increases in \( c \in [-1,1] \), which is shown in Lemma 3.3. Thus, we have \( \cos \theta_k(c) \in [\frac{1}{2},1], \cos \theta_k(c) - \frac{2\pi}{3} \in [-\frac{1}{2},\frac{1}{2}], \cos \theta_k(c) - \frac{4\pi}{3} \in [-1,\frac{1}{2}] \) and hence we obtain

\[
0 \leq A_2(c,k) \leq \frac{1}{4} \leq A_1(c,k) \leq \frac{3}{4} \leq A_0(c,k) \leq 1.
\]
for any \( c \in [-1,1] \) and \( k=0,1,2,\ldots,\ell-1 \). Furthermore, we have the followings:

- \( A_2(c,k) = 0 \) if and only if \((c,k) = (-1, \frac{\pi}{2})\).
- \( A_2(c,k) = \frac{1}{4} \) if and only if \((c,k) = (1,0)\).
- \( A_1(c,k) = \frac{1}{4} \) if and only if \((c,k) = (1,0)\).
- \( A_1(c,k) = \frac{3}{4} \) if and only if \((c,k) = (-1, \frac{\pi}{2})\).
- \( A_0(c,k) = \frac{3}{4} \) if and only if \((c,k) = (-1, \frac{\pi}{2})\).
- \( A_0(c,k) = 1 \) if and only if \((c,k) = (0,0)\).

Note that \( A_0(c,k) \) increases in \( c \in [-1,1] \), \( A_1(c,k) \) decreases in \( c \in [-1,1] \) and \( A_2(c,k) \) increases in \( c \in [-1,1] \) for a fixed \( k=0,1,2,\ldots,\ell-1 \).

Due to Lemma 3.3 and Remark 3.2, we obtain the followings:

**Lemma 3.4.** For any \( c \in [-1,1] \) and \( k=0,1,2,\ldots,\ell-1 \), the solutions to the equation \( D_0(k,\lambda) - c = 0 \) on \( \sqrt{\lambda} \) are given by \( \lambda \in \mathbb{R} \) satisfying \( \sqrt{\lambda} = \beta_j(c,k) + 2(n-1)\pi, \ j = 1,2,\ldots,12, \ n \in \mathbb{N}, \) where

\[
\beta_1(c,k) = \arccos \sqrt{A_0(c,k)}, \quad \beta_3(c,k) = \arccos \sqrt{A_2(c,k)}, \quad \beta_5(c,k) = \arccos(-\sqrt{A_1(c,k)}), \\
\beta_2(c,k) = \arccos \sqrt{A_1(c,k)}, \quad \beta_4(c,k) = \arccos(-\sqrt{A_2(c,k)}), \quad \beta_6(c,k) = \arccos(-\sqrt{A_0(c,k)}), \\
\beta_7(c,k) = 2\pi - \beta_6(c,k), \quad \beta_8(c,k) = 2\pi - \beta_5(c,k), \quad \beta_9(c,k) = 2\pi - \beta_4(c,k), \\
\beta_{10}(c,k) = 2\pi - \beta_3(c,k), \quad \beta_{11}(c,k) = 2\pi - \beta_2(c,k), \quad \beta_{12}(c,k) = 2\pi - \beta_1(c,k).
\]

Moreover, we have \( \beta_1(c,k) \in [0, \frac{\pi}{4}], \beta_2(c,k) \in [\frac{\pi}{4}, \frac{\pi}{2}], \beta_3(c,k) \in [\frac{\pi}{2}, \pi], \beta_4(c,k) \in [\pi, \frac{3\pi}{2}], \beta_5(c,k) \in [\frac{3\pi}{2}, \frac{5\pi}{4}], \beta_6(c,k) \in [\frac{5\pi}{4}, \pi] \) for any \( c \in [-1,1] \) and \( k=0,1,2,\ldots,\ell-1 \).

We next examine the zeroes of \( D(k,\lambda) - c \) for \( c \in [-1,1] \). To this end, we need to recall standard Rouché’s theorem and estimates for \( e^{[3\sqrt{\lambda}]} \) on some lines inside the \( \sqrt{\lambda} \)-plane:

**Theorem 3.1.** (Rouché’s theorem) Let \( D \) be a region in \( C, \) \( C \) the boundary of \( D. \) If \( f \) and \( g \) are analytic on \( \overline{D} \) and \( |f(z)| < |g(z)| \) holds true for \( z \in C, \) then \( f + g \) and \( g \) have the same number of zeroes inside \( D. \)

**Lemma 3.5.** ([15, Lemma 3.6 and Remark 3.7]) 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 \( e^{[3\sqrt{\lambda}]} < C_p |\cos \sqrt{\lambda} + p| \) on \( C_\pm(n) := \{ \lambda \in \mathbb{C} | \sqrt{\lambda} = \pm ni + t, \ t \in \mathbb{R} \} \) for any \( n \geq n_0(p). \)

(ii) For a fixed \( p \in (-1,1), \) there exists some constant \( C_p > 0 \) such that \( e^{[3\sqrt{\lambda}]} < C_p |\cos \sqrt{\lambda} + p| \) on \( C(n,q) := \{ \lambda \in \mathbb{C} | \sqrt{\lambda} = n\pi + \arccos\cos q + ti, \ -n \leq t \leq n \} \) 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 \( e^{[3\sqrt{\lambda}]} < C_p'' |\cos \sqrt{\lambda} + p| \) on \( C(n,q) \) for each \( q \in (-1,1) \setminus \{ p, -p \} \) and \( n \in \mathbb{N}. \)
In order to set ahead, we also need to prepare the followings:

**Lemma 3.6.** For \( k = 0, 1, 2, \ldots, \ell - 1 \), we have

\[
D(k, \lambda) = D_0(k, \lambda) + O\left(\frac{e^{b|\lambda|}}{|\lambda|}\right) \quad \text{as} \quad |\lambda| \to \infty.
\]

**Proof.** We recall the asymptotics as \( |\lambda| \to \infty \) of the fundamental solutions to (1.1) from [18]:

\[
\begin{align*}
\theta(1, \lambda) &= \cos \sqrt{\lambda} + \frac{1}{2\sqrt{\lambda}} \int_0^1 (\sin \sqrt{\lambda} + \sin \sqrt{\lambda}(1 - 2t)) q(t) dt + O\left(\frac{e^{b|\lambda|}}{|\lambda|}\right), \\
\varphi'(1, \lambda) &= \cos \sqrt{\lambda} + \frac{1}{2\sqrt{\lambda}} \int_0^1 (\sin \sqrt{\lambda} + \sin \sqrt{\lambda}(1 - 2t)) q(t) dt + O\left(\frac{e^{b|\lambda|}}{|\lambda|}\right).
\end{align*}
\]

These formulas yield

\[
\Delta^2(\lambda) = \cos^2 \sqrt{\lambda} + O\left(\frac{e^{2b|\lambda|}}{|\lambda|}\right) \quad \text{and} \quad \Delta_-(\lambda) = O\left(\frac{e^{b|\lambda|}}{|\lambda|}\right) \quad \text{as} \quad |\lambda| \to \infty.
\]

Substituting these into (3.1), we obtain our desired formula. \( \square \)

For real sequences \( \{a_n\}_{n=1}^{\infty} \) and \( \{b_n\}_{n=1}^{\infty} \) satisfying \( a_n < b_n \) for every \( n \in \mathbb{N} \), we define segments

\[
\begin{align*}
C^+(b_n) &= \{ \lambda \in \mathbb{C} \mid \sqrt{\lambda} = b_n + ti, \quad -n \leq t \leq n \}, \\
C^-(a_n) &= \{ \lambda \in \mathbb{C} \mid \sqrt{\lambda} = a_n - ti, \quad -n \leq t \leq n \}, \\
C^\times(a_n, b_n) &= \{ \lambda \in \mathbb{C} \mid \sqrt{\lambda} = ni + b_n + t(a_n - b_n), \quad 0 \leq t \leq 1 \}, \\
C^+(a_n, b_n) &= \{ \lambda \in \mathbb{C} \mid \sqrt{\lambda} = -ni + a_n + t(b_n - a_n), \quad 0 \leq t \leq 1 \}
\end{align*}
\]

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 \( n \in \mathbb{N} \). Moreover, let \( \Omega(a_n, b_n) \) be the region surrounded by \( C(a_n, b_n) \) for each \( n \in \mathbb{N} \). Using Theorem 3.1, Lemmas 3.5 and 3.6, we obtain the followings:

**Lemma 3.7.** (i) Let \( c \in (-1, 1) \). Then, there exists some \( n_0(c) \in \mathbb{N} \) satisfying the followings:

- The function \( D(k, \lambda) - c \) has exactly one zero, counted with the multiplicities, inside each domain \( \Omega(n \pi, n \pi + \frac{\pi}{2}) \), \( \Omega(n \pi + \frac{\pi}{2}, n \pi + \frac{3\pi}{2}) \), \( \Omega(n \pi + \frac{\pi}{2}, n \pi + \frac{\pi}{2}), \Omega(n \pi + \frac{\pi}{2}, n \pi + \frac{3\pi}{2}) \), \( \Omega(n \pi + \frac{\pi}{2}, n \pi + \frac{\pi}{2}) \) and \( \Omega(n \pi + n^2 + \frac{\pi}{2}, (n+1)\pi) \) for all \( n > n_0 \).

- The function \( D(k, \lambda) - c \) has 6n zeroes, counted with the multiplicities, inside \( \Omega(-n\pi, n\pi) \) for all \( n > n_0 \).

- There are no other zeroes.
3.2. Putting Lemma 3.6 that on each contour for a large $n > n_0$, we have the following:

- The function $D(k, \lambda) - 1$ has exactly 2 zeroes, counted with the multiplicities, inside each domain $\Omega((n - \frac{1}{2})\pi - \frac{\pi}{12}, (n - \frac{1}{2})\pi + \frac{\pi}{12})$ for all $n > n_0$.

- The function $D(k, \lambda) - 1$ has exactly $1 + 6n$ zeroes, counted with the multiplicities, inside $\Omega((- (n\pi + \frac{\pi}{12}), n\pi + \frac{\pi}{12})$ for all $n > n_0$.

- There are no other zeroes.

(iii) There is some $n_0 \in \mathbb{N}$ satisfying the followings:

- The function $D(k, \lambda) + 1$ has exactly 2 zeroes, counted with the multiplicities, inside each domain $\Omega((n - \frac{1}{2})\pi - \frac{\pi}{12}, (n - \frac{1}{2})\pi + \frac{\pi}{12})$ and $\Omega((n - \frac{5}{6})\pi - \frac{\pi}{12}, (n - \frac{5}{6})\pi + \frac{\pi}{12})$ for all $n > n_0$.

- The function $D(k, \lambda) + 1$ has exactly $6n$ zeroes, counted with the multiplicities, inside $\Omega((- (n\pi + \frac{\pi}{12}), n\pi + \frac{\pi}{12})$ for all $n > n_0$.

- There are no other zeroes.

Proof. Let us give the proof of (i). We first see that $D_0(k, \lambda)$ satisfies (i) by virtue of Lemma 3.2. Putting $X_1(c, k) = \sqrt{A_0(c, k)}$, $X_2(c, k) = -\sqrt{A_0(c, k)}$, $X_3(c, k) = \sqrt{A_1(c, k)}$, $X_4(c, k) = -\sqrt{A_1(c, k)}$, $X_5(c, k) = \sqrt{A_2(c, k)}$ and $X_6(c, k) = -\sqrt{A_2(c, k)}$, we have

$$D_0(k, \lambda) - c = \frac{36}{\cos \frac{\pi k}{6}} \prod_{j=1}^{6} (\cos \sqrt{\lambda} + X_j(c, k)). \quad (3.3)$$

For $p = X_1(c, k), X_2(c, k), \ldots, X_6(c, k)$, it turns out by Lemma 3.5 that there exist some constants $M_1(c, k), M_2(c, k), \ldots, M_6(c, k) > 0$ such that $e^{[3\sqrt{\lambda}]} < M_j(c, k)|\cos \sqrt{\lambda} + X_j(c, k)|$ on each contour $C(n\pi, n\pi + \frac{\pi}{3})$, $C(n\pi + \frac{\pi}{3}, n\pi + \frac{2\pi}{3})$, $C(n\pi + \frac{2\pi}{3}, n\pi + \frac{\pi}{3})$, $C(n\pi + \frac{\pi}{3}, n\pi + 2\pi)$, $C(n\pi + \frac{\pi}{3}, n\pi + 3\pi)$ and $C(n\pi + \frac{\pi}{3}, (n+1)\pi)$ for all $n \in \mathbb{N}$ and each $j = 1, 2, \ldots, 6$. Let us give the proof of this claim. It follows by Remark 3.2 that $p \in (-1, 1) \setminus \{ \pm \frac{\pi}{3}, \pm \frac{\pi}{3}, 0 \}$. It follows by Lemma 3.5 (ii) that $e^{[3\sqrt{\lambda}]} < C_p|\cos \sqrt{\lambda} + p|$ on $C(n, q)$ for $q = 0, \pm \frac{\pi}{3}, \pm \frac{\pi}{3}, \pm 1 \in (-1, 1) \setminus \{ p, -p \}$ and $n \in \mathbb{N}$. This combined with Lemma 3.5 (i) means the existence of our desired $M_1(c, k), M_2(c, k), \ldots, M_6(c, k) > 0$. Thus, it follows by Lemma 3.6 that

$$|(D(k, \lambda) - c) - (D_0(k, \lambda) - c)| = \mathcal{O}\left( \left| \frac{e^{[3\sqrt{\lambda}]}|\lambda|}{|\sqrt{\lambda}|} \right| \right) = \mathcal{O}\left( \frac{1}{|\lambda|} \right) \prod_{j=1}^{6} |\cos \sqrt{\lambda} + X_j(c, k)|$$

on each contour for a large $n \in \mathbb{N}$. So, it turns out on each contour for a large $n \in \mathbb{N}$ that

$$|(D(k, \lambda) - c) - (D_0(k, \lambda) - c)| = \mathcal{O}\left( \frac{1}{|\lambda|} \right) |D_0(k, \lambda) - c|$$
owing to (3.3). Therefore, we obtain the statement (i) as a result of Rouché’s theorem.

In a similar way, we obtain the statements (ii) and (iii) using Lemmas 3.5 (i) and (iii).

Proof of Theorem 1.2. Since \( \theta(1, \lambda) \) and \( \varphi(1, \lambda) \) are real for any \( \lambda \in \mathbb{R} \), we see that \( D(k, \lambda) \) is also real for a \( \lambda \in \mathbb{R} \). This combined with Lemmas 3.2 and 3.7 implies that \( D(k, \lambda) - 1 \) and \( D(k, \lambda) + 1 \) has only the real zeroes. Let \( \lambda_{k,0}^+, \lambda_{k,1}^+, \lambda_{k,2}^+, \cdots, (\lambda_{k,1}^-, \lambda_{k,1}^+, \lambda_{k,3}^+, \cdots) \) be the zeroes of \( D(k, \lambda) - 1 \) (\( D(k, \lambda) + 1 \), respectively), which are arranged in the increasing order. Furthermore, Lemma 3.7 yields \( \lambda_{k,0}^+, \lambda_{k,1}^- < \lambda_{k,1}^+, \lambda_{k,2}^-, \cdots, \lambda_{k,n}^- \), and hence we have \( \sigma_{ac}(H_k) = \bigcup_{j=1}^{\infty} [\lambda_{k,j-1}, \lambda_{k,j}] \). Moreover, Remarks 3.1 implies that \( \lambda_{k,2j}^+ \neq \lambda_{k,2j}^- \) \( \lambda_{k,2j-1} \neq \lambda_{k,2j+1} \) holds true for \( k = 1, 2, \cdots, l - 1 \) \( k \in \{0, 1, 2, \cdots, \ell - 1\} \setminus \{\frac{N}{2}\} \).

4 Asymptotic analysis

Assume that \( N = 2 \ell - 1 \) or \( N = 2 \ell \) for a fixed \( \ell \in \mathbb{N} \). In this section, we obtain the asymptotic behavior of \( \{\lambda_{k,j}^\pm\} \) for each \( k = 0, 1, 2, \cdots, \ell - 1 \). In order to state the key lemma of this section, we recall \( \beta_1(c, k), \cdots, \beta_{12}(c, k) \) introduced in Lemma 3.4 and prepare notations. We define

\[
\begin{align*}
&u_{k,12n+j}^- = 2n\pi + u_{k,j}^- + u_{k,0}^+, \quad u_{k,12n}^+ = 2n\pi + u_{k,0}^+, \quad u_{k,12n+12}^- = 2n\pi + u_{k,12}^- \quad \text{for} \quad n = 0, 1, 2, \cdots, 11, \quad j = 1, 2, \cdots, 11,
\end{align*}
\]

where

\[
\begin{align*}
&u_{k,0}^- = 0, \quad u_{k,2}^+ = \lambda_{k,1}^+, \quad u_{k,2}^- = \lambda_{k,1}^-, \quad u_{k,4}^- = \beta_4(1, k), \quad u_{k,4}^+ = \beta_5(1, k), \\
&u_{k,6}^- = \beta_6(1, k), \quad u_{k,6}^+ = 2\pi - u_{k,6}^-, \quad u_{k,8}^- = 2\pi - u_{k,8}^+, \quad u_{k,8}^+ = 2\pi - u_{k,8}^-, \\
&u_{k,10}^+ = 2\pi - u_{k,10}^-, \quad u_{k,10}^- = 2\pi - u_{k,10}^+, \quad u_{k,12}^- = 2\pi - u_{k,12}^+, \\
&u_{k,12}^+ = 2\pi - u_{k,12}^-,
\end{align*}
\]

These notations are needed to describe the zeroes of \( D_0(k, \lambda) - 1 \) and \( D_0(k, \lambda) + 1 \).

Lemma 4.1. We have \( \{\sqrt{\lambda} \mid D_0(k, \lambda) - 1 = 0\} = \{u_{k,0}^+, u_{k,2}^+, u_{k,4}^+, u_{k,6}^+, u_{k,8}^+, \cdots\} \) and \( \{\sqrt{\lambda} \mid D_0(k, \lambda) + 1 = 0\} = \{u_{k,1}^+, u_{k,3}^+, u_{k,5}^+, u_{k,7}^+, u_{k,9}^+, \cdots\} \).

Proof. Putting \( c = 1 \) or \( c = -1 \) in the statement of Lemma 3.4, we obtain the conclusion.

We put \( q_0 = \int_0^1 q(x) dx \) and define \( q \) is even if and only if \( q(x) = q(1-x) \) for almost every \( x \in (0, 1) \). The key point of this section is the following:
Lemma 4.2. (I) (a) Let $k \neq 0$. Then, for $p = 1, 2, 3, 4, 5, 6$, we have
\[2 \sqrt{\lambda_{k,12n+2p}^\pm} = 2u_{k,12n+2p}^\pm + \frac{q_0}{u_{k,12n+2p}^\pm} + o \left( \frac{1}{n^2} \right) \quad \text{as } n \to \infty.\]

(b) Let $k = 0$. Then, we have the followings:
\[2 \sqrt{\lambda_{0,12n+p}^\pm} = 2u_{0,12n+p}^\pm + \frac{q_0}{u_{0,12n+p}^\pm} + o \left( \frac{1}{n} \right) \quad \text{as } n \to \infty \quad \text{for } p = 6, 12.\]
\[2 \sqrt{\lambda_{0,12n+p}^\pm} = 2u_{0,12n+p}^\pm + \frac{q_0}{u_{0,12n+p}^\pm} + o \left( \frac{1}{n^2} \right) \quad \text{as } n \to \infty \quad \text{for } p = 2, 4, 8, 10.\]

(II) (a) Let $k = \frac{N}{3}$ and $q$ be not even. Then, for $p = 1, 3, 5, 7, 9, 11$, we have
\[2 \sqrt{\lambda_{\frac{N}{3},12n+p}^\pm} = 2u_{\frac{N}{3},12n+p}^\pm + \frac{q_0}{u_{\frac{N}{3},12n+p}^\pm} + o \left( \frac{1}{n^2} \right) \quad \text{as } n \to \infty.\]

(b) Let $k \neq \frac{N}{3}$ or $q$ be even. Then, for $p = 1, 3, 5, 7, 9, 11$, we have
\[2 \sqrt{\lambda_{k,12n+p}^\pm} = 2u_{k,12n+p}^\pm + \frac{q_0}{u_{k,12n+p}^\pm} + o \left( \frac{1}{n^2} \right) \quad \text{as } n \to \infty.\]

Remark 4.1. Especially, we note that $u_{0,12n}^\pm = 2n\pi, u_{0,12n+2}^\pm = \frac{4}{3} + 2n\pi, u_{0,12n+4}^\pm = \frac{5}{3} \pi + 2n\pi, u_{0,12n+6}^\pm = \pi + 2n\pi, u_{0,12n+8}^\pm = \frac{4}{3} \pi + 2n\pi, u_{0,12n+10}^\pm = \frac{5}{3} \pi + 2n\pi, u_{0,12n+12}^\pm = 2\pi + 2n\pi, u_{\frac{N}{3},12n+1}^\pm = \frac{5}{6} \pi + 2n\pi, u_{\frac{N}{3},12n+3}^\pm = \frac{7}{6} \pi + 2n\pi, u_{\frac{N}{3},12n+5}^\pm = \frac{9}{6} \pi + 2n\pi, u_{\frac{N}{3},12n+7}^\pm = \frac{11}{6} \pi + 2n\pi, u_{\frac{N}{3},12n+9}^\pm = \frac{3}{2} \pi + 2n\pi, u_{\frac{N}{3},12n+11}^\pm = \frac{13}{6} \pi + 2n\pi$ for every $n \in \mathbb{N}$ owing to Remark 3.2.

Let us start the discussion to prove this lemma. To this end, we consider the equation $D(k,\lambda) = 1$. It follows by a straightforward calculation that $D(k,\lambda) = 1$ is equivalent to
\[
\Delta^6 - \left( \frac{3}{2} + \frac{\Delta^2}{9} \right) \Delta^4 + \left( \frac{9}{16} + \frac{\Delta^2}{18} \right) \Delta^2 - \frac{1}{144} \left( 3 + 2\cos \frac{2\pi k}{N} + 4\cos \frac{\pi k}{N} + \Delta^2 \right) = 0. \tag{4.1}
\]
We solve this equation on $\Delta^2$ utilizing the Viète’s method. Putting $\Delta^2 = z + \frac{1}{2} \left( \frac{3}{2} + \frac{\Delta^2}{9} \right)$, we see that (4.1) is equivalent to
\[
z^3 - \left( \frac{3}{16} + \frac{\Delta^2}{18} + \frac{\Delta^4}{243} \right) z - \frac{f_k(1)}{288} - \frac{\Delta^2}{9} \left( \frac{1}{8} + \frac{\Delta^2}{54} + \frac{2\Delta^4}{2187} \right) = 0, \tag{4.2}
\]
where $f_k(c)$ is the one defined in Lemma 3.3: $f_k(c) = 8c^2 + 8c - 7$. If $q \equiv 0$, then we have $\Delta_- = 0$ and hence we can make sure that (4.2) is the same as (3.2). We define
\[
p_+ = \frac{3}{16} + \frac{\Delta^2}{18} + \frac{\Delta^4}{243}, \quad q_+ = \frac{f_k(1)}{288} + \frac{\Delta^2}{9} \left( \frac{1}{8} + \frac{\Delta^2}{54} + \frac{2\Delta^4}{2187} \right). \tag{4.3}
\]
Let $D_k^+$ be the discriminant for (4.2), i.e., $D_k^+ = 4p_+^3 - 27q_+^2$. Its signature is as follows:
Lemma 4.3. If \( k = 0 \), then we have \( D_k^+ = 0 \). Otherwise, namely, if \( k = 1, 2, \cdots, \ell - 1 \), then \( D_k^+ > 0 \).

Proof. It turns out by substituting (4.3) for the \( \lambda \) where \( t \), we have

\[
\begin{align*}
-D_k^+ &= -D_0^+ + 27 \left\{ t_k^2 + 2t_k \left( \frac{1}{32} + A(\lambda) \right) \right\},
\end{align*}
\]

where \( t_k = \frac{1}{36} \left( \cos \frac{k\pi}{\ell} - 1 \right) \left( \cos \frac{k\pi}{\ell} + 2 \right), A(\lambda) = \frac{\Delta^2}{9} \left( \frac{1}{8} + \frac{\Delta^2}{54} + \frac{2\Delta^4}{2187} \right) \) and

\[
-D_0^+ = -4 \left( \frac{3}{16} + \frac{\Delta^2}{18} + \frac{\Delta^4}{243} \right)^3 + 27 \left\{ \frac{1}{32} + \frac{\Delta^2}{9} \left( \frac{1}{8} + \frac{\Delta^2}{54} + \frac{2\Delta^4}{2187} \right) \right\}^2.
\]

It follows by straightforward but hard calculations, i.e., expanding (4.5), that \( D_k^+ > 0 \). Thus, we obtain the first statement.

We next show the second statement. Assume that \( k = 1, 2, \cdots, \ell - 1 \). Substituting \( D_0^+ = 0 \) for (4.4), we obtain

\[
-D_k^+ = 27 \left\{ t_k^2 + 2t_k \left( \frac{1}{32} + A(\lambda) \right) \right\} = 27 \left\{ t_k + \frac{1}{32} + A(\lambda) \right\}^2 - \left( \frac{1}{32} + A(\lambda) \right)^2.
\]

We claim that \( t_k \in (\frac{-1}{18}, 0) \). Since \( \cos \frac{7k\pi}{\ell} \in (0, 1) \) for \( k = 1, 2, \cdots, \ell - 1 \), we consider \( g(x) = \frac{7k}{36} (x - 1)(x + 2) \) for \( x \in (0, 1) \). Since \( g(x) = \frac{1}{36} \left\{ (x + \frac{1}{2})^2 - \frac{9}{4} \right\} \), we obtain \( g(x) \in (-\frac{1}{18}, 0) \). Hence, we have \( t_k \in (\frac{-1}{18}, 0) \). Since \( A(\lambda) \geq 0 \), we see that \( \sup_{X \in (-\frac{1}{18}, 0)} F(X) = F(0) = 0 \), where

\[
F(X) = X^2 + 2 \left( \frac{1}{32} + A(\lambda) \right) X
\]

for \( X \in (-\frac{1}{18}, 0) \). Thus, we obtain \( F(X) < 0 \) for all \( X \in (-\frac{1}{18}, 0) \). This implies that \( -D_k^+ < 0 \) and hence \( D_k^+ > 0 \). \( \Box \)

Owing to this lemma, we see that (4.2) has the different 3 solutions \( z_{0,k}^+ (\lambda) \), \( z_{1,k}^+ (\lambda) \) and \( z_{2,k}^+ (\lambda) \) in the case where \( k = 1, 2, \cdots, \ell - 1 \), where

\[
z_{m,k}^+ (\lambda) := 2 \sqrt{\frac{p_+}{3}} \cos \left\{ \frac{1}{3} \arccos \left( \frac{3q_+}{2p_+} \sqrt{\frac{3}{p_+}} \right) - \frac{2\pi m}{3} \right\}, \quad m = 0, 1, 2.
\]

We obtain the asymptotic behavior for these solutions as follows:

Lemma 4.4. Let \( k = 1, 2, \cdots, \ell - 1 \). Then, we have

\[
z_{m,k}^+ (\lambda) = \frac{1}{2} \cos \left( \frac{1}{3} \arccos \frac{f_k(1)}{9} - \frac{2\pi m}{3} \right) + O(\Delta^2)
\]

as \( \lambda \to +\infty \).
Proof. According to Taylor’s theorem, there exist some \( \theta_1, \theta_2 \in (0, 1) \) such that 
\[
\frac{1}{1+x} = 1 - x + \frac{x^2}{1+x} + \frac{3x^3}{(1+\theta_1 x)^3} \text{ and } \frac{1}{\sqrt{1+x}} = 1 - \frac{x}{2} + \frac{3x^2}{8(1+\theta_2 x)^{3/2}}.
\]
Thus, we obtain \( \frac{1}{2p_+} = \frac{8}{3} + O(\Delta^2) \) and \( \frac{3}{p_+} = 4 + O(\Delta^2) \) and hence
\[
\frac{3q_+}{2p_+} = \frac{f_k(1)}{36} + O(\Delta^2) \quad \text{and} \quad \frac{3q_+}{2p_+} = \frac{3}{p_+} = \frac{f_k(1)}{9} + O(\Delta^2)
\]
as \( \lambda \to +\infty \). Recall \( \frac{f_k(1)}{9} \in (-1, 1) \) for \( k = 1, 2, \ldots, \ell - 1 \) from the proof of Lemma 3.3. Owing to Taylor’s theorem, for \( a, x \in (-1, 1) \), there exists some \( \theta \in (0, 1) \) such that
\[
\arccos(a + x) = \arccos a - \frac{x}{\sqrt{1-a^2}} - \frac{a + \theta x}{\{1-(a+\theta x)^2\}^{3/2}} x^2.
\]
Thus, we see that
\[
\gamma_{k+} := \frac{1}{3} \arccos \left( \frac{3q_+}{2p_+} \sqrt{\frac{3}{p_+}} \right) = \frac{1}{3} \arccos \frac{f_k(1)}{9} + O(\Delta^2)
\]
as \( \lambda \to +\infty \). Moreover, we obtain
\[
\cos \left( \gamma_{k+} - \frac{2\pi m}{3} \right) = \cos \left\{ \alpha_k + O(\Delta^2) \right\} \cos \frac{2\pi m}{3} + \sin \left\{ \alpha_k + O(\Delta^2) \right\} \sin \frac{2\pi m}{3}
\]
as \( \lambda \to +\infty \), where \( \alpha_k = \theta_k(1) \). Here, we note that \( \theta_k(c) \) is the one defined in Lemma 3.3. Since we obtain \( \cos(\alpha_k + O(\Delta^2)) = \cos \alpha_k + O(\Delta^2) \), \( \sin(\alpha_k + O(\Delta^2)) = \sin \alpha_k + O(\Delta^2) \) and
\[
\sqrt{\frac{3}{p_+}} = \frac{1}{2} + O(\Delta^2) \text{ as } \lambda \to +\infty \text{ owing to Taylor’s theorem, we obtain}
\]
\[
z^+_{mk}(\lambda) = 2 \left( \frac{1}{4} + O(\Delta^2) \right) \left[ \cos \frac{2\pi m}{3} \left( \cos \alpha_k + O(\Delta^2) \right) + \sin \frac{2\pi m}{3} \left( \sin \alpha_k + O(\Delta^2) \right) \right]
\]
\[
= \frac{1}{2} \cos \frac{2\pi m}{3} \cos \alpha_k + \frac{1}{2} \sin \frac{2\pi m}{3} \sin \alpha_k + O(\Delta^2)
\]
\[
= \frac{1}{2} \cos \left( \alpha_k - \frac{2\pi m}{3} \right) + O(\Delta^2)
\]
as \( \lambda \to +\infty \). This implies our goal. \( \square \)

Remark 4.2. Since \( \Delta^2 = z + \frac{1}{3} \left( \frac{3}{2} + \frac{\Delta^2}{\lambda} \right) \), the solutions \( \Delta_{k,0}, \Delta_{k,1}, \Delta_{k,2} \) to the cubic equation (4.1) on \( \Delta^2 \) satisfy
\[
\Delta_{k,m}(\lambda) = \frac{1}{2} \cos \left( \frac{1}{3} \arccos \frac{f_k(1)}{9} - \frac{2\pi m}{3} \right) + O(\Delta^2) \quad \text{as } \lambda \to +\infty \text{ for } m = 0, 1, 2.
\]
Before we give the proof of Lemma 4.2 (I)(a), we note a remark:
Remark 4.3. Let $k = 0, 1, 2, \cdots, \ell - 1$. It follows by Lemma 3.7 (ii) and (iii) that there are a large $n_0 \in \mathbb{N}$ satisfying the followings for any $n > n_0$:

\[
\sqrt{\lambda_{k,6n}^+ - \frac{n_0}{2}} \in \Omega \left( \left( n - \frac{5}{6} \right) \pi - \frac{\pi}{12}, \left( n - \frac{5}{6} \right) \pi + \frac{\pi}{12} \right),
\]

\[
\sqrt{\lambda_{k,6n-4}^+} \in \Omega \left( \left( n - \frac{2}{3} \right) \pi - \frac{\pi}{12}, \left( n - \frac{2}{3} \right) \pi + \frac{\pi}{12} \right),
\]

\[
\sqrt{\lambda_{k,6n-3}^+} \in \Omega \left( \left( n - \frac{1}{2} v \right) \pi - \frac{\pi}{12}, \left( n - \frac{1}{2} v \right) \pi + \frac{\pi}{12} \right),
\]

\[
\sqrt{\lambda_{k,6n-2}^+} \in \Omega \left( \left( n - \frac{1}{3} \right) \pi - \frac{\pi}{12}, \left( n - \frac{1}{3} \right) \pi + \frac{\pi}{12} \right),
\]

\[
\sqrt{\lambda_{k,6n-1}^+} \in \Omega \left( \left( n - \frac{1}{6} \right) \pi - \frac{\pi}{12}, \left( n - \frac{1}{6} \right) \pi + \frac{\pi}{12} \right),
\]

\[
\sqrt{\lambda_{k,6n}^+} \in \Omega \left( (n+1) \pi - \frac{\pi}{12}, (n+1) \pi + \frac{\pi}{12} \right).
\]

This implies that

\[
\left| \sqrt{\lambda_{k,n}^+ - u_{k,n}^+} \right| < \frac{\pi}{6}
\]

for $n > n_0$ and $k = 0, 1, 2, \cdots, \ell - 1$. Furthermore, we have $\sqrt{\lambda_{k,n}^+} = O(n)$ as $n \to \infty$.

Proof of Lemma 4.2 (I)(a). Assume that $k = 1, 2, \cdots, \ell - 1$. Let us recall from [7] that $\chi(\lambda) = \sqrt{\lambda - \frac{q_0}{2}} + o(1)$ as $|\lambda| \to \infty$, where $\Delta(\lambda) = \cos \chi(\lambda)$. We give the proof for $p = 6$. Since $\sqrt{\lambda_{k,12}^+}$ is close to $u_{k,12n+12}^+ = 2(n+1)\pi \pm \arccos \sqrt{A_0(1,k)}$ in the sense of Remark 4.3, we have $m = 0$. Remark 4.2 combined with $\Delta(\lambda_{k,12n+12}^+) = \cos \chi(\lambda_{k,12n+12}^+) = \cos \alpha_k + O(\Delta^2)$ implies that

\[
\cos 2\chi(\lambda_{k,12n+12}^+) = \cos \alpha_k + O(\Delta^2) \quad (4.7)
\]
as $|\lambda| \to \infty$ and

\[
\chi(\lambda_{k,12n+12}^+) = \sqrt{\lambda_{k,12n+12}^+} - \frac{q_0}{2 \sqrt{\lambda_{k,12n+12}^+}} + o(1) \quad (4.8)
\]
as $n \to \infty$. Putting $\chi(\lambda_{k,12n+12}^+) = a_{k,12n+12}^+ + ib_{k,12n+12}^+$ and $a_{k,12n+12}^+, b_{k,12n+12}^+ \in \mathbb{R}$, we see that

\[
a_{k,12n+12}^+ = \sqrt{\lambda_{k,12n+12}^+} - \frac{q_0}{2 \sqrt{\lambda_{k,12n+12}^+}} + o(1) \quad \text{and} \quad b_{k,12n+12}^+ = \frac{o(1)}{\lambda_{k,12n+12}^+}
\]
as $n \to \infty$. Thus, we have

\[
\cos 2\chi(\lambda_{k,12n+12}^+) = \cos 2a_{k,12n+12}^+ \cosh 2b_{k,12n+12}^+ - i \sin 2a_{k,12n+12}^+ \sinh b_{k,12n+12}^+.
\]
This combined with (4.7) means that \( \cos 2\alpha^\pm_{k,12n+12} \to \cos \alpha_k \) as \( n \to \infty \). It follows by \( u^\pm_{k,12n+12} = 2(n+1)\pi \pm \arccos \sqrt{A_0(1,k)} \) that
\[
\cos 2u^\pm_{k,12n+12} = 2\cos^2(\arccos \sqrt{A_0(1,k)}) - 1 = 2 \left( \frac{1}{2} \cos \alpha_k + \frac{1}{2} \right) - 1 = \cos \alpha_k
\]
and hence
\[
\cos \left( 2\sqrt{\lambda^\pm_{k,12n+12} - \frac{q_0}{\lambda^\pm_{k,12n+12}} + \frac{o(1)}{\lambda^\pm_{k,12n+12}}} \right) - 2\cos^2 \left( \frac{1}{2} \right) \to 0
\]
as \( n \to \infty \). Since \( \sqrt{\lambda^\pm_{k,n} - u^\pm_{k,n}} < \frac{\pi}{n} \) for a large \( n \in \mathbb{N} \) (see Remark 4.3), we have
\[
2\sqrt{\lambda^\pm_{k,12n+12} - \frac{q_0}{\lambda^\pm_{k,12n+12}} + \frac{o(1)}{\lambda^\pm_{k,12n+12}} - 2u^\pm_{k,12n+12} \to 0
\]
as \( n \to \infty \). This combined with \( \sqrt{\lambda^\pm_{k,n} - u^\pm_{k,n}} < \frac{\pi}{n} \) implies that \( \epsilon^\pm_{k,12n+12} \to 0 \) as \( n \to \infty \), where
\[
\epsilon^\pm_{k,12n+12} = 2\sqrt{\lambda^\pm_{k,12n+12} - 2u^\pm_{k,12n+12} + \frac{q_0}{\lambda^\pm_{k,12n+12}} - o(1)} \left( \frac{1}{n^2} \right)
\]
as \( n \to \infty \). Let us show that \( \epsilon^\pm_{k,12n+12} = o\left( \frac{1}{n^2} \right) \) as \( n \to \infty \). Since it follows by (4.8) that
\[
\chi(\lambda^\pm_{k,12n+12}) = \sqrt{\lambda^\pm_{k,12n+12} - \frac{q_0}{2u^\pm_{k,12n+12}} + o(1)} \left( \frac{1}{n^2} \right)
\]
as \( n \to \infty \). So, we have
\[
2\chi(\lambda^\pm_{k,12n+12}) = 2\epsilon^\pm_{k,12n+12} + \epsilon^\pm_{k,12n+12}.
\]
It follows by Taylor’s theorem that
\[
\cos 2\chi(\lambda^\pm_{k,12n+12}) = \cos(2u^\pm_{k,12n+12} + \epsilon^\pm_{k,12n+12})
\]
\[
= \cos 2u^\pm_{k,12n+12} - (\sin 2u^\pm_{k,12n+12})\epsilon^\pm_{k,12n+12} + O((\epsilon^\pm_{k,12n+12})^2)
\]
\[
= \cos \alpha_k - (\sin 2u^\pm_{k,12n+12})\epsilon^\pm_{k,12n+12} + O((\epsilon^\pm_{k,12n+12})^2).
\]
This combined with (4.7) and \( \Delta^2 = o\left( \frac{1}{n^2} \right) \) as \( |\lambda| \to \infty \) yields
\[
O\left( \frac{1}{n^2} \right) = - (\sin 2u^\pm_{k,12n+12})\epsilon^\pm_{k,12n+12} + O((\epsilon^\pm_{k,12n+12})^2)
\]
as \( n \to \infty \). Noticing \( \alpha_k \in (0, \frac{\pi}{2}) \) and hence \( \sin^2 2u^\pm_{k,12n+12} = 1 - \cos^2 2u^\pm_{k,12n+12} = 1 - \cos^2 \alpha_k \neq 0 \), we obtain \( \epsilon^\pm_{k,12n+12} = o\left( \frac{1}{n^2} \right) \) as \( n \to \infty \). Therefore, we obtain
\[
2\sqrt{\lambda^\pm_{k,12n+12} = 2u^\pm_{k,12n+12} + \frac{q_0}{u^\pm_{k,12n+12}} = o\left( \frac{1}{n^2} \right)}
\]
as \( n \to \infty \). In a similar way, we obtain our asymptotic for \( p=1,2,3,4,5 \). Hence, we conclude that the statement (I)(a) holds true.
We next consider the proof of Lemma 4.2 (I)(b).

Proof of Lemma 4.2 (I)(b). Assume that \( k = 0 \). Then, (4.2) implies that

\[
 z^3 - \left( \frac{3}{16} + \frac{\Delta^2}{18} + \frac{\Delta^4}{243} \right) z - \left\{ \frac{1}{32} + \frac{\Delta^2}{9} \left( \frac{1}{8} + \frac{\Delta^2}{54} + \frac{2\Delta^4}{2187} \right) \right\} = 0. \tag{4.9}
\]

Since we have made sure that \( D_0^+ = 0 \) in the proof of Lemma 4.3, this equation has a multiple root. In fact, (4.9) is factored as follows:

\[
 \left\{ z - \left( \frac{1}{2} + \frac{\Delta^2}{27} \right) \right\} \left\{ z + \left( \frac{1}{4} + \frac{\Delta^2}{27} \right) \right\}^2 = 0.
\]

Since \( \Delta^2 = \frac{1}{2} \left( \frac{3}{2} + \Delta^2 \right) \), we see that \( \Delta^2 = 1 + \frac{\Delta^2}{9} \) (whose multiplicity is 1) and \( \frac{1}{4} \) (whose multiplicity is 2) solve (4.1) in the case of \( k = 0 \). Furthermore, this implies that

\[
 \Delta^2 (\lambda_{0,12n+6}^\pm) = \Delta^2 (\lambda_{0,12n+12}^\pm) = 1 + \frac{\Delta^2}{9} (\lambda_{0,12n+12}^\pm),
\]

\[
 \Delta^2 (\lambda_{0,12n+2}) = \Delta^2 (\lambda_{0,12n+4}) = \Delta^2 (\lambda_{0,12n+8}) = \Delta^2 (\lambda_{0,12n+10}) = \frac{1}{4}
\]

for all \( n \in \mathbb{N} \).

Let us show our result for \( p = 12 \). Putting \( \Delta (\lambda) = \cos \chi (\lambda) \), we see by \( \Delta^2 (\lambda_{0,12n+12}^\pm) = 1 + \frac{\Delta^2}{9} (\lambda_{0,12n+12}^\pm) \) and \( \Delta_-(\lambda) = o \left( \frac{1}{\sqrt{n}} \right) \) as \( |\lambda| \to \infty \) and \( \lambda \in \mathbb{R} \) that

\[
 \cos 2\chi (\lambda_{0,12n+12}^\pm) = 1 + \frac{2}{9} \Delta^2 (\lambda_{0,12n+12}^\pm) = 1 + O (\Delta^2) = 1 + o \left( \frac{1}{\lambda_{0,12n+12}^\pm} \right) = 1 + o \left( \frac{1}{n^2} \right) \tag{4.10}
\]

as \( n \to \infty \). Recall that \( \chi (\lambda_{0,12n+12}^\pm) = \sqrt{\lambda_{0,12n+12}^\pm} - \frac{2q_0}{\sqrt{\lambda_{0,12n+12}^\pm}} + o \left( \frac{1}{\lambda_{0,12n+12}^\pm} \right) \) as \( n \to \infty \) from [7].

Thus, putting \( \Re (\lambda_{0,12n+12}^\pm) = a_{0,12n+12}^\pm \) and \( \Im (\lambda_{0,12n+12}^\pm) = b_{0,12n+12}^\pm \), we have

\[
 a_{0,12n+12}^\pm = \sqrt{\lambda_{0,12n+12}^\pm} - \frac{q_0}{2 \sqrt{\lambda_{0,12n+12}^\pm}} + o \left( \frac{1}{\lambda_{0,12n+12}^\pm} \right) \quad \text{and} \quad b_{0,12n+12}^\pm = \frac{o \left( 1 \right)}{\lambda_{0,12n+12}^\pm}
\]

as \( n \to \infty \). Thus, \( \cos 2\chi (\lambda_{0,12n+12}^\pm) \to 1 \) as \( n \to \infty \) implies that \( \cos (2a_{0,12n+12}^\pm) \to 1 \) as \( n \to \infty \). Since \( \cos 2u_{0,12n+12} \equiv 1 \), we have \( \cos 2a_{0,12n+12}^\pm - \cos 2u_{0,12n+12}^\pm \to 0 \) as \( n \to \infty \). Since it follows by Remark 4.3 that \( |\sqrt{\lambda_{0,12n+12}^\pm} - u_{0,12n+12}^\pm| < \frac{2}{5} \), this yields \( 2a_{0,12n+12}^\pm - 2u_{0,12n+12}^\pm \to 0 \) as \( n \to \infty \). This implies that

\[
 2 \sqrt{\lambda_{0,12n+12}^\pm} - \frac{q_0}{\sqrt{\lambda_{0,12n+12}^\pm}} + o \left( \frac{1}{\lambda_{0,12n+12}^\pm} \right) - 2u_{0,12n+12}^\pm \to 0
\]
as \( n \to \infty \). Hence, we see that

\[
e^{\pm}_{0,12n+12} := 2\sqrt{\lambda_{0,12n+12}^2 - 2u_{0,12n+12}^2 - \frac{q_0}{u_{0,12n+12}} + o\left(\frac{1}{n^2}\right)} \to 0
\]

as \( n \to \infty \). It follows by Taylor’s theorem that

\[
\cos 2\chi(\lambda_{0,12n+12}^\pm) = \cos(2u_{0,12n+12}^\pm + e_{0,12n+12}^\pm) = 1 - \frac{1}{2}(e_{0,12n+12}^\pm + o((e_{0,12n+12}^\pm)^2)) \quad (4.11)
\]

as \( n \to \infty \). This combined with (4.10) means that \( e_{0,12n+12}^\pm = o\left(\frac{1}{n^2}\right) \) as \( n \to \infty \). Thus, we obtain the statement in Lemma 4.2 (I)(b) for \( p = 12 \). In a similar way, we have our results for \( p = 6 \).

Let us show our result for \( p = 2 \). We put \( e_{0,12n+2}^\pm = 2\sqrt{\lambda_{0,12n+2}^2 - 2u_{0,12n+2}^2 - \frac{q_0}{u_{0,12n+2}} + o\left(\frac{1}{n^2}\right)} \) as \( n \to \infty \). In a similar way to the case of \( p = 12 \), we see that \( e_{0,12n+2}^\pm \to 0 \) as \( n \to \infty \). Moreover, in a similar way to the case of \( p = 12 \), we obtain \( \cos 2\chi(\lambda_{0,12n+2}^\pm) = -\frac{1}{2} = -\frac{1}{2} + o\left(\frac{1}{n^2}\right) \) for all \( \alpha > 0 \) and

\[
\cos 2\chi(\lambda_{0,12n+2}^\pm) = -\frac{1}{2} - \frac{\sqrt{3}}{2} e_{0,12n+2}^\pm + o\left((e_{0,12n+2}^\pm)^2\right)
\]

as \( n \to \infty \) instead of (4.10) and (4.11). Thus, we obtain \( e_{0,12n+2}^\pm = o\left(\frac{1}{n^2}\right) \) as \( n \to \infty \) for all \( \alpha > 0 \). Putting \( \alpha = 2 \), we obtain the desired result. The proof for \( p = 4, 8, 10 \) is similar to the one for \( p = 2 \).

Now that we have obtained the asymptotics for zeroes of \( D(k,\lambda) = 1 \) in the sense of Lemma 4.2 (I), we next examine the asymptotics for zeroes of \( D(k,\lambda) = -1 \), which is equivalent to

\[
\Delta^6 - \left(\frac{3}{2} + \frac{\Delta^2}{9}\right) \Delta^4 + \left(\frac{9}{16} + \frac{\Delta^2}{18}\right) \Delta^2 - \frac{1}{144}\left(3 + 2\cos \frac{2\pi k}{\nu} - 4\cos \frac{\pi k}{\nu} + \Delta^2\right) = 0. \quad (4.12)
\]

Putting \( \Delta^2 = z + \left(\frac{1}{2} + \frac{\Delta^2}{2\nu}\right) \), this is moreover equivalent to

\[
z^3 - \left(\frac{3}{16} + \frac{\Delta^2}{18} + \frac{\Delta^4}{243}\right) z - \frac{f_k(-1)}{288} \frac{\Delta^2}{9} \left(\frac{1}{8} + \frac{\Delta^2}{54} + \frac{2\Delta^4}{2187}\right) = 0. \quad (4.13)
\]

Here, we recall \( f_k(-1) = 8c_k^2 - 8c_k - 7 \) and \( c_k = \cos \frac{\pi k}{\nu} \) for \( k = 0, 1, \cdots, \ell - 1 \). We consider the discriminant \( D_k^{-} = D_k^{-}(\lambda) = 4p_3^2 - 27q_3^2 \) for (4.13), where

\[
p_3 = \frac{3}{16} + \frac{\Delta^2}{18} + \frac{\Delta^4}{243}, \quad q_3 = \frac{f_k(-1)}{288} \frac{\Delta^2}{9} \left(\frac{1}{8} + \frac{\Delta^2}{54} + \frac{2\Delta^4}{2187}\right). \quad (4.14)
\]

Then, we have the followings on this discriminant:
Lemma 4.5. (i) If \( k = \frac{N}{3} \) and \( q \) is even, then we have \( D_k^- = 0 \).

(ii) Assume that \( k \neq \frac{N}{3} \) or \( q \) is not even. Then, for \( k = 0, 1, \ldots, \ell - 1 \), there exists some \( \lambda_0 \in \mathbb{R} \) such that \( D_k^- > 0 \) for any \( \lambda \geq \lambda_0 \).

Proof. Let \( q_{\omega-} \) be the \( q_- \) for \( k = \frac{N}{3} \). Then, we have \( q_{\omega-} - q_- = \frac{9}{288} - \frac{1}{288}(8c_k^2 - 8c_k - 7) = -\frac{1}{288}(8c_k^2 - 8c_k + 2) = \frac{1}{288}\{8(c_k - \frac{1}{2}) - 8(c_k^2 - \frac{1}{4})\} = \frac{1}{36}(c_k - \frac{1}{2})\{1 - (c_k + \frac{1}{2})\} = -\frac{1}{36}(c_k - \frac{1}{2})^2 \). So, we see that \( z^3 - p - z - q_- = 0 \) is equivalent to \( z^3 - p - z - q_{\omega-} - \frac{1}{36}(c_k - \frac{1}{2})^2 = 0 \). This is why we have

\[
D_k^- = D_k^- - 27\left( c_k - \frac{1}{2} \right)^2 \left( \frac{1}{36} c_k - \frac{1}{2} \right)^2 + \frac{q_{\omega-}}{18} \right)
\]

(4.15)

It follows by straightforward calculations that \( D_k^- = \frac{3}{64} \Delta^2 + \frac{1}{144} \Delta^4 + \frac{1}{2916} \Delta^6 \). Thus, we see that \( D_k^- = 0 \) if \( q \) is even. Hence, we obtain the statement (i). Moreover, we have \( D_k^- > 0 \) if \( q \) is not even. Assume that \( k \neq \frac{N}{3} \) or \( q \) is not even. Then, (4.15) implies that

\[
D_k^- > -27 \left( c_k - \frac{1}{2} \right)^2 \left\{ \frac{1}{36} \left( c_k - \frac{1}{2} \right)^2 + \frac{q_{\omega-}}{18} \right\}
\]

\[
= -27 \left( c_k - \frac{1}{2} \right)^2 \left\{ \frac{1}{36^2} \left( c_k - \frac{1}{2} \right)^2 + \frac{1}{18} \left\{ -\frac{1}{32} + \frac{\Delta^2}{9} \left( \frac{1}{8} + \frac{\Delta^2}{54} + \frac{2\Delta^4}{2187} \right) \right\} \right\}
\]

\[
= -\frac{1}{48} \left( c_k - \frac{1}{2} \right)^2 \left\{ \left( c_k - \frac{1}{2} \right)^2 - \frac{9}{4} + 8\Delta^2 \left( \frac{1}{8} + \frac{\Delta^2}{54} + \frac{2\Delta^4}{2187} \right) \right\}.
\]

(4.16)

Since \( \left( c_k - \frac{1}{2} \right)^2 - \frac{9}{4} \in [-\frac{9}{4}, -2] \) for \( k = 0, 1, 2, \ldots, \ell - 1 \) and \( \Delta_\pm \to 0 \) as \( |\lambda| \to \infty \), (4.16) implies the existence of our desired \( \lambda_0 \).

Let us give the proof of Lemma 4.2 (II)(b).

Proof of Lemma 4.2 (II)(b). First, we consider the case where \( k = \frac{N}{3} \) and \( q \) is even. Then, we have \( \Delta_- = 0 \). Substituting \( k = \frac{N}{3} \) and \( \Delta_- = 0 \) into (4.13), we have

\[
z^3 - \frac{3}{16}z + \frac{1}{32} = 0,
\]

which is equivalent to \( (z + \frac{1}{2})(z - \frac{1}{2})^2 = 0 \). Thus, we see that the solutions to the cubic equation (4.12) on \( \Delta^2 \) are \( \Delta^2 = 0, \frac{3}{8} \) (The multiplicity of 0 is 1. The multiplicity of \( \frac{3}{8} \) is 2).

This implies that \( \Delta^2(\lambda_{\pm,1+12n}^\pm) = \frac{3}{8}, \Delta^2(\lambda_{\pm,3+12n}^\pm) = 0, \Delta^2(\lambda_{\pm,5+12n}^\pm) = \frac{3}{8}, \Delta^2(\lambda_{\pm,7+12n}^\pm) = \frac{3}{8}, \Delta^2(\lambda_{\pm,9+12n}^\pm) = 0, \Delta^2(\lambda_{\pm,11+12n}^\pm) = \frac{3}{8} \) for each \( n \in \mathbb{N} \). In a similar way to the proof of Lemma 4.2 (I)(b), we obtain our assertion.
Next, we consider the case where \( k \neq \frac{N}{3} \). Since it follows by Lemma 4.5 (ii) that \( D_+ > 0 \) for a large \( \lambda \), (4.13) has the distinct three roots expressed as the Vieté’s solutions if \( \lambda \) is large:

\[
z_{m,k}^- = 2 \left( \frac{p_-}{3} \right)^{1/2} \cos \left\{ \frac{1}{3} \arccos \left( \frac{3q_-}{2p_-} \sqrt{\frac{3}{p_-}} \right) - \frac{2\pi m}{3} \right\}, \quad m = 0, 1, 2. \tag{4.17}
\]

We stress that \( f_k(-1) \in (-9, 9) \) for \( k \neq \frac{N}{3} \) (see the proof of Lemma 3.3). In a similar way to Lemma 4.4, we have

\[
z_{m,k}^- = \frac{1}{2} \cos \left( \frac{1}{3} \arccos \left( \frac{f_k(-1)}{9} \right) - \frac{2\pi m}{3} \right) + O(\Delta^2)
\]

and hence the solutions to the cubic equation (4.12) on \( \Delta^2 \) satisfy

\[
\Delta^2 = \frac{1}{2} + \frac{1}{2} \cos \left( \frac{1}{3} \arccos \left( \frac{f_k(-1)}{9} \right) - \frac{2\pi m}{3} \right) + O(\Delta^2)
\]

as \( \lambda \to +\infty \). Thus, we obtain the statement of Lemma 4.2 (II)(b) in a similar to the proof of Lemma 4.2 (I)(a).

**Proof of Lemma 4.2 (II)(a).** Let us suppose that \( k = \frac{N}{3} \) and \( q \) is not even. According to Taylor’s theorem, there exist some \( \theta_1, \theta_2 \in (0, 1) \) such that \( \frac{1}{1+x} = 1-x+\frac{x^2}{(1+\theta_2)(1+\theta_2)^2} \) and \( \sqrt{1+x} = 1-\frac{x}{2}+\frac{3x^2}{8(1+\theta_2)^3} \). Thus, we have \( \frac{1}{2p_-} = \frac{8}{3} - \frac{27}{12} \Delta^2 + O(\Delta^4) \) and \( \sqrt{\frac{3}{p_-}} = 4 - \frac{16}{3} \Delta^4 + O(\Delta^6) \) as \( \lambda \to +\infty \). So, we see that

\[
\frac{3q_-}{2p_-} = \left( \frac{8}{3} - \frac{27}{12} \Delta^2 + O(\Delta^4) \right) \left( \frac{f_k(-1)}{96} + \frac{\Delta^2}{24} + O(\Delta^4) \right)
\]

\[
= \frac{f_k(-1)}{36} + \frac{96-f_k(-1)}{864} \Delta^2 + O(\Delta^4)
\]

as \( \lambda \to +\infty \). Since \( f_\frac{N}{3}(-1) = -9 \), we have

\[
\frac{3q_-}{2p_-} \sqrt{\frac{3}{p_-}} = -1 + a \Delta^2 + O(\Delta^4)
\]

as \( \lambda \to \infty \), where \( a = \frac{411}{2724} > 0 \). It follows by Taylor’s theorem that

\[
\arccos \left( \frac{3q_-}{2p_-} \sqrt{\frac{3}{p_-}} \right) = \arccos \left( -1 + a \Delta^2 \right) - \frac{O(\Delta^4)}{\sqrt{2a \Delta^2 - a^2 \Delta^4}} - \frac{-1 + a \Delta^2 + O(\Delta^4)}{-2a \Delta^2 + O(\Delta^4)} O(\Delta^8)
\]

\[
= \arccos \left( -1 + a \Delta^2 \right) + O(\Delta^3) \tag{4.18}
\]
as $\lambda \to \infty$. We put $\xi(\lambda) = \arccos(-1 + a\Delta^2) - \pi$. Let us show that $\xi(\lambda) = \mathcal{O}(\Delta_-)$ as $\lambda \to \infty$. First, we see that $\xi(\lambda) \to 0$ due to $\Delta_-(\lambda) \to 0$ as $\lambda \to +\infty$. It follows by the Taylor’s theorem that there exists some $\theta \in (0, 1)$ satisfying

$$-1 + a\Delta_- = \cos(\arccos(-1 + a\Delta^2_\ast)) = \cos(\pi + \xi) = -\cos\xi = -1 + \frac{1}{2} \xi^2 + \frac{\cos(\theta \cdot \xi)}{4!} \xi^4. \quad (4.19)$$

This combined with $a > 0$ implies that $\xi(\lambda) = \mathcal{O}(\Delta_-)$ as $\lambda \to \infty$. Thus, (4.18) yields

$$\arccos\left(\frac{3q_-}{2p_-} \sqrt{\frac{3}{p_-}}\right) = \pi + \mathcal{O}(\Delta_-)$$

as $\lambda \to \infty$. Hence, we have

$$\cos\left(\frac{1}{3} \arccos\left(\frac{3q_-}{2p_-} \sqrt{\frac{3}{p_-}}\right) - \frac{2\pi m}{3}\right) = \cos\left(\frac{\pi}{3} - \frac{2\pi m}{3}\right) - \sin\left(\frac{\pi}{3} - \frac{2\pi m}{3}\right) \cdot \mathcal{O}(\Delta_-) + \mathcal{O}(\Delta_-^2)$$

as $\lambda \to \infty$. This combined with $\sqrt{\frac{p_-}{\lambda}} = \frac{1}{2} + \mathcal{O}(\Delta_-^2)$ as $\lambda \to \infty$ yields

$$z_{\nu, k}^n = \frac{1}{2} \cos\left(\frac{\pi}{3} - \frac{2\pi m}{3}\right) - \frac{1}{2} \sin\left(\frac{\pi}{3} - \frac{2\pi m}{3}\right) \mathcal{O}(\Delta_-) + \mathcal{O}(\Delta_-^2)$$

as $\lambda \to \infty$. Since $\Delta^2 = z + \left(\frac{1}{2} + \frac{\Delta^2}{27}\right)$, we see that the solutions to the cubic equation (4.12) on $\Delta^2$ in the case where $k = \frac{n}{4}$ and $q$ is not even are given by

$$\Delta^2 = \frac{1}{2} + \frac{1}{2} \cos\left(\frac{\pi}{3} - \frac{2\pi m}{3}\right) - \frac{1}{2} \sin\left(\frac{\pi}{3} - \frac{2\pi m}{3}\right) \mathcal{O}(\Delta_-) + \mathcal{O}(\Delta_-^2)$$

as $\lambda \to \infty$. Putting $\Delta(\lambda) = \cos\chi(\lambda)$, we have

$$\cos^2\chi(\lambda) = \cos\left(\frac{\pi}{3} - \frac{2\pi m}{3}\right) - \sin\left(\frac{\pi}{3} - \frac{2\pi m}{3}\right) \mathcal{O}(\Delta_-) + \mathcal{O}(\Delta_-^2) \quad \text{as } \lambda \to \infty. \quad (4.20)$$

Let us show the result for $p = 1$. For $\lambda_{\frac{n}{2}, 1+12n}^\alpha$ we have $m = 0$ and hence

$$\cos^2\chi(\lambda_{\frac{n}{2}, 1+12n}^\alpha) = \frac{1}{2} \sqrt{\frac{3}{2}} \mathcal{O}(\Delta_-) + \mathcal{O}(\Delta_-^2) \quad (4.21)$$

as $\lambda \to \infty$. In a similar way to the proof of Lemma 4.2 (I)(b), we have

$$\cos^2\chi(\lambda_{\frac{n}{2}, 1+12n}^\alpha) = \frac{1}{2} - \cos(2\pi \lambda_{\frac{n}{2}, 1+12n}^\alpha) + \mathcal{O}\left((\epsilon_{n, 1+12n}^\alpha)^2\right) \quad (4.22)$$

as $\lambda \to \infty$, where $\epsilon_{n, 1+12n}^\alpha = \sqrt{\lambda_{\frac{n}{2}, 1+12n}^\alpha} - \frac{\epsilon_{n, 1+12n}^0}{\sqrt{\lambda_{\frac{n}{2}, 1+12n}^\alpha}} + \mathcal{O}\left(1\right) - \nu_{1+12n} \to 0$. It follows by (4.21) and (4.22) that $\epsilon_{n, 1+12n}^\alpha = o(\Delta_-) = o\left(\sqrt{\lambda_{\frac{n}{2}, 1+12n}^\alpha}\right) = o\left(\frac{1}{n}\right)$ as $n \to \infty$. Thus, we obtain the result for $p = 1$. In a similar way, we see that the results for $p = 3, 5, 7, 9, 11$ are valid.
Proof of Theorem 1.3(i). We obtain the statement (a) in Theorem 1.3 (i) due to Lemma 4.2 (I)(a). Moreover, we obtain (1.4) using Lemma 4.2 (I)(b). Thus, we show (1.5) and (1.6).

First, we have \(\lambda_{0,12n+1}^+ = (\mu_{0,12n+1}^0)^2 + q_0 + o(1)\) as \(n \to \infty\) by Lemma 4.2 (I)(b). Let \(\{\eta_n\}_{n=0}^\infty\) be the zeroes of \(\Delta(\lambda)\), where \(\Delta(\lambda)\) implies the derivative of \(\Delta(\lambda)\). Moreover, we recall the \(j\)th gap \((\lambda_{2j-1}, \lambda_{2j})\) for \(-\frac{d^2}{dx^2} + q\) in \(L^2(\mathbb{R})\). Then, we have \(\eta_{2n} = 4n^2 \pi^2 + q_0 + \ell^2(n)\), \(\lambda_{2n} = n^2 \pi^2 + q_0 + |\dot{q}_n| + O\left(\frac{1}{n}\right)\), and \(\lambda_{2n-1} = n^2 \pi^2 + q_0 - |\dot{q}_n| + O\left(\frac{1}{n}\right)\) as \(n \to \infty\), where \(\dot{q}_n = \int_0^1 q(x) e^{2\pi inx} dx\) (see [5] and [8]). Thus, we have \(\epsilon_{0,12n}^+ \to 0\) and \(\epsilon_{2n}^+ = |\dot{q}_{2n}| + O\left(\frac{1}{n}\right)\) as \(n \to \infty\), where \(\epsilon_{0,12n}^+ = \lambda_{0,12n}^+ - \eta_{2n}\) and \(\epsilon_{2n}^+ = \lambda_{4n} - \eta_{2n}\). It follows by Taylor’s theorem that

\[
\Delta(\lambda_{0,12n}^+) = \Delta(\eta_{2n}) + \Delta(\eta_{2n}) \epsilon_{0,12n}^+ + \frac{\Delta(\eta_{2n})}{2} (\epsilon_{0,12n}^+)^2 + \frac{\Delta(\eta_{2n})}{6} (\epsilon_{0,12n}^+)^3 (1 + O(\epsilon_{0,12n}^+)) \quad (4.23)
\]

as \(n \to \infty\). Here, we recall from [10, 14] that

\[
\Delta(\lambda) = 1 + O\left(\frac{1}{n}\right), \quad \Delta(\lambda) = O\left(\frac{1}{n}\right), \quad \Delta(\lambda) = -\frac{1 + O(\frac{1}{n})}{(4n \pi)^2}, \quad \Delta(\lambda) = O\left(\frac{1}{n^4}\right) \quad (4.24)
\]

as \(\sqrt{\lambda} = 2n \pi + O\left(\frac{1}{n}\right)\) and \(n \to \infty\). These combined with (4.23) and \(\Delta(\eta_{2n}) = 0\) yield that

\[
\Delta(\lambda_{0,12n}^+) = \Delta(\eta_{2n}) + A_{0,12n}^+ \quad (4.25)
\]

where

\[
A_{0,12n}^+ = \frac{\Delta(\eta_{2n})}{2} (\epsilon_{0,12n}^+)^2 \left(1 + O\left(\frac{\epsilon_{0,12n}^+}{n^2}\right)\right) = -\frac{1 + O(\frac{1}{n})}{2(4n \pi)^2} (\epsilon_{0,12n}^+)^2 \left(1 + O\left(\frac{\epsilon_{0,12n}^+}{n^2}\right)\right)
\]

as \(n \to \infty\). On the other hand, we utilize Taylor’s theorem for \(\Delta(\lambda_{2n}^+)\). Then, it follows by \(\Delta(\eta_{2n}) = 0\) that

\[
1 = \Delta(\lambda_{2n}^+) = \Delta(\eta_{2n}) + A_{2n}^+ \quad (4.26)
\]

where

\[
A_{2n}^+ = \frac{\Delta(\eta_{2n})}{2} (\epsilon_{2n}^+)^2 + \frac{\Delta(\eta_{2n})}{6} (\epsilon_{2n}^+)^2 (1 + O(\epsilon_{2n}^+)) \quad \text{as} \quad n \to \infty.
\]

Due to (4.24), we have

\[
A_{2n}^+ = \frac{\Delta(\eta_{2n})}{2} (\epsilon_{2n}^+)^2 \left(1 + O\left(\frac{\epsilon_{2n}^+}{n^2}\right)\right) = -\frac{1 + O(\frac{1}{n})}{2(4n \pi)^2} (\epsilon_{2n}^+)^2 \left(1 + O\left(\frac{\epsilon_{2n}^+}{n^2}\right)\right) \quad (4.27)
\]

as \(n \to \infty\). It follows by (4.25) and (4.26) that

\[
\Delta(\lambda_{0,12n}^+) = 1 + A_{0,12n}^+ - A_{2n}^+ = 1 + B_{2n}^+ + o\left(\frac{1}{n^3}\right) \quad (4.28)
\]
as $n \to \infty$, where $B^{+}_{2n} = \frac{(\epsilon^{+}_{2n})^2 - (\epsilon^{+}_{0,12n})^2}{2(4n\pi)^2} = o \left(\frac{1}{n^2}\right)$ as $n \to \infty$. Let us recall

$$\Delta_-(\lambda) = \frac{q_{s,0,2n} + O \left(\frac{1}{n}\right)}{4n\pi}, \quad \Delta_+(\lambda) = -\frac{q_{s,1,2n} + O \left(\frac{1}{n}\right)}{(4n\pi)^2}, \quad \Delta_0(\lambda) = -\frac{q_{s,2,2n} + O \left(\frac{1}{n}\right)}{(4n\pi)^3}$$

(4.29)

as $\sqrt{\lambda} = 2n\pi + O \left(\frac{1}{n}\right)$ and $n \to \infty$ from [14]. Substituting (4.28), (4.29) and $\lambda = \lambda^{+}_{0,12n}$ into

$$D(0,\lambda) = 36\Delta^6 - (54 + 4\Delta^-)\Delta^4 + \left(2\Delta^- + \frac{81}{4}\right)\Delta^2 - \frac{1}{4}(5 + \Delta^-),$$

(4.30)

which follows by (1.2), we obtain

$$36 \left(1 + B^{+}_{2n} + o \left(\frac{1}{n^3}\right)^6 \right) - \left(54 + 4\left(q_{s,0,2n} + O \left(\frac{1}{n}\right)\right)^2\right) \left(1 + B^{+}_{2n} + o \left(\frac{1}{n^3}\right)^4\right)$$

$$+ \left\{2\left(q_{s,0,2n} + O \left(\frac{1}{n}\right)\right)^2 + \frac{81}{4}\right\} \left(1 + B^{+}_{2n} + o \left(\frac{1}{n^3}\right)\right) - \frac{1}{4} \left(9 + \left(q_{s,0,2n} + O \left(\frac{1}{n}\right)\right)^2\right) = 0.$$

Expanding each term of this equality and using $B^{+}_{2n} = o \left(\frac{1}{n^2}\right)$ as $n \to \infty$, we have

$$\frac{81}{4} B^{+}_{2n} - 3\left(q_{s,0,2n} + O \left(\frac{1}{n}\right)\right)^2 + o \left(\frac{1}{n^3}\right) = 0$$

as $n \to \infty$. Thus, we obtain

$$(\epsilon^{+}_{2n})^2 - (\epsilon^{+}_{0,12n})^2 - \frac{8}{27} \left(q_{s,0,2n} + O \left(\frac{1}{n}\right)\right)^2 + o \left(\frac{1}{n^3}\right) = 0$$

as $n \to \infty$ by the definition of $B^{+}_{2n}$. This combined with $\epsilon^{+}_{2n} = |q_{2n}| + O \left(\frac{1}{n}\right)$ as $n \to \infty$ implies

$$(\epsilon^{+}_{0,12n})^2 = |q_{2n}|^2 - \frac{8}{27} q_{s,0,2n} + o \left(\frac{1}{n}\right)$$

as $n \to \infty$.

Since $q_{2n} = 4n^2 + q_0 + O \left(\frac{1}{n}\right)$ and $\epsilon^{+}_{0,12n} = \lambda^{+}_{0,12n} - q_{2n}$, this implies (1.5) if $\epsilon^{+}_{0,12n} \geq 0$ for a large $n \in \mathbb{N}$.

Let us show $\epsilon^{+}_{0,12n} \geq 0$ for a large $n$. Differentiating (4.30) with respect to $\lambda$, we have

$$\dot{D}(0,\lambda)$$

$$= 216\Delta^5\dot{\Delta} - 8\Delta_+\dot{\Delta_+}\Delta^4 - 4(54 + 4\Delta_-^2)\Delta^3\dot{\Delta} + 4\Delta_+\dot{\Delta_+}\Delta^2 + 2\Delta_+\dot{\Delta} \left(2\Delta_-^2 + \frac{81}{4}\right) - \frac{1}{2}\Delta_+\dot{\Delta_-}.$$

(4.31)
Furthermore, we have
\[
\dot{D}(0, \lambda) = 216 \Delta^4 \Delta^2 + 216 \Delta^5 \Delta - 8 \Delta^2 \Delta^4 - 8 \Delta \Delta^4 - 32 \Delta \Delta^2 \Delta^3 \\
-32 \Delta \Delta^2 \Delta^3 - 4(54 + 4 \Delta^2) \cdot (3 \Delta^2 \Delta^2 + \Delta^3 \Delta) \\
+ 4 \Delta^2 \Delta^2 + 4 \Delta \Delta \Delta^2 + 8 \Delta \Delta \Delta \\
+ 8 \Delta \Delta \Delta + 2 \left( 2 \Delta^2 + \frac{81}{4} \right) (\Delta^2 + \Delta \Delta) - \frac{1}{2} \Delta^2 - \frac{1}{2} \Delta \Delta.
\] (4.32)

Let \( \lambda_{0,12n} \) be the zero of \( \dot{D}(0, \lambda) \) in the interval \([\lambda_{0,12n}, \lambda_{0,12n}^+] \) for every \( n \in \mathbb{N} \). Substituting (4.24), (4.29) and \( \lambda = \lambda_{0,12n} \) into (4.32), we obtain
\[
\dot{D}(0, \lambda_{0,12n}) = - \frac{81 s_{2n}}{2(4n\pi)^2} + o \left( \frac{1}{n^2} \right) \quad \text{as } n \to \infty.
\] (4.33)
as \( n \to \infty \). We put \( s_{2n} = \eta_{2n} - \lambda_{0,12n} \). Here, we recall \( \{ \eta_n \}_{n=0}^{\infty} \) be the zeroes of \( \Delta(\lambda) \). It follows by Taylor’s theorem that
\[
\dot{D}(0, \eta_{2n}) = \dot{D}(0, \lambda_{0,12n}) s_{2n} (1 + O(s_{2n})) \quad \text{as } n \to \infty.
\]
Substituting (4.33) into this, we have
\[
\dot{D}(0, \eta_{2n}) = - \frac{81 s_{2n}}{2(4n\pi)^2} + o \left( \frac{s_{2n}}{n^2} \right) \quad \text{as } n \to \infty.
\] (4.34)
On the other hand, it follows by putting \( \lambda = \eta_{2n} \) in (4.31) that
\[
\dot{D}(0, \eta_{2n}) = \Delta_{-}(\eta_{2n}) \Delta_{-}^{'}(\eta_{2n}) \left( -8 \Delta^4(\eta_{2n}) + 4 \Delta^2(\eta_{2n}) - \frac{1}{2} \right),
\]
owing to \( \Delta(\eta_{2n}) = 0 \). Inserting (4.24) and (4.29) into this, we have
\[
\dot{D}(0, \eta_{2n}) = \frac{9}{2} \cdot \frac{q_{s,2n}}{4n\pi} \cdot \frac{q_{c,12n}}{(4n\pi)^2} + O \left( \frac{1}{n^4} \right) \quad \text{as } n \to \infty.
\] (4.35)
Comparing (4.34) and (4.35), we obtain
\[
s_{2n} = - \frac{q_{s,2n} q_{c,12n}}{36n\pi} + O \left( \frac{1}{n^2} \right) \to 0 \quad \text{as } n \to \infty.
\]
This implies that \( \eta_{2n} \) and \( \lambda_{0,12n} \) are very close for a large \( n \in \mathbb{N} \). This moreover implies that \( \epsilon_{0,12n}^+ = \lambda_{0,12n}^+ - \eta_{2n} \geq 0 \) for a large \( n \in \mathbb{N} \). Thus, we obtain (1.5) for \( \lambda_{0,12n+12}^+ \). As for \( \lambda_{0,12n+12}^- \), we obtain (1.5) in a similar way. Similarly, we have (1.6).

Finally, let us give the proof of Theorem 1.3 (ii).

\[ \Box \]
Proof of Theorem 1.3 (ii). Since (1.7) directly follows by Lemma 4.2 (II)(b). Thus, it suffices to show that (1.8) and (1.9). Let us assume that $k = \frac{N}{q}$ and $q$ is not even. First, we enhance the proof of Lemma 4.2 (II)(a). Due to (4.20) and $\xi = \arccos(-1+a\Delta^2) - \pi$, we have

$$
\begin{align*}
\cos\left(\frac{1}{3}\arccos\left(\frac{3q-2p\sqrt{p}}{p}\right) - \frac{2m\pi}{3}\right) \\
= \cos\left\{\frac{1}{3}\arccos\left(-1+a\Delta^2\right) - \frac{2m\pi}{3} + O(\Delta^3)\right\} \\
= \cos\left(\frac{\pi + \xi(\lambda)}{3} - \frac{2m\pi}{3}\right)\cos O(\Delta_0^2) - \sin\left(\frac{\pi + \xi(\lambda)}{3} - \frac{2m\pi}{3}\right)\sin O(\Delta_0^3) \\
\end{align*}
$$

as $n \to \infty$. Note that there exists some $\theta_1, \theta_2 \in (0, 1)$ satisfying

$$
\begin{align*}
\cos \frac{\xi(\lambda)}{3} &= 1 - \frac{1}{2} \left(\frac{\xi(\lambda)}{3}\right)^2 + \cos \theta_1 \frac{\xi(\lambda)}{3} 4! \\
\sin \frac{\xi(\lambda)}{3} &= \frac{\xi(\lambda)}{3} - \sin \theta_2 \frac{\xi(\lambda)}{3} 3! \\
\end{align*}
$$

These combined with (4.36) and $\xi(\lambda) = O(\Delta_0)$ as $n \to \infty$ yield

$$
\begin{align*}
\cos\left(\frac{1}{3}\arccos\left(\frac{3q-2p\sqrt{p}}{p}\right) - \frac{2m\pi}{3}\right) \\
= \left\{\cos\left(\frac{1-2m}{3}\pi\right)\cos\frac{\xi(\lambda)}{3} - \sin\left(\frac{1-2m}{3}\pi\right)\sin\frac{\xi(\lambda)}{3}\right\} \left(1 + O(\Delta_0^6)\right) \\
- \left\{\sin\left(\frac{1-2m}{3}\pi\right)\cos\frac{\xi(\lambda)}{3} + \cos\left(\frac{1-2m}{3}\pi\right)\sin\frac{\xi(\lambda)}{3}\right\} \left(1 + O(\Delta_0^6)\right) \left(1 + O(\Delta^3)\right) \\
= \left[\cos\left(\frac{1-2m}{3}\pi\right)\left(1 - \frac{\xi^2(\lambda)}{18} + O(\xi^4(\lambda))\right) - \sin\left(\frac{1-2m}{3}\pi\right)\left(\frac{\xi(\lambda)}{3} + O(\xi^3(\lambda))\right)\right] \\
- \sin\left(\frac{1-2m}{3}\pi\right)\left(1 - \frac{\xi^2(\lambda)}{18} + O(\xi^4(\lambda))\right) O(\Delta_0^3) + O(\Delta^4) \\
= \left\{\cos\left(\frac{1-2m}{3}\pi\right) - \sin\left(\frac{1-2m}{3}\pi\right) O(\Delta_0^2)\right\} \left(1 - \frac{\xi^2(\lambda)}{18}\right) \\
- \sin\left(\frac{1-2m}{3}\pi\right)\left(\frac{\xi(\lambda)}{3} + O(\xi^3(\lambda))\right) + O(\Delta^4) \\
\end{align*}
$$

as $n \to \infty$. Due to (4.20), we have

$$
\xi^2(\lambda) = \frac{2a\Delta^2}{1 + O(\xi^2(\lambda))} \quad \text{as} \quad n \to \infty.
$$
There exists some \( \theta_5 \in (0,1) \) satisfying \( \frac{1}{1+x} = 1 - x + \frac{2}{(1+\theta_5 x)^2} x^2 \) by Taylor’s theorem. So, we see that \( z^2(\lambda) = 2a\Delta^2 + \Delta^2 \cdot \mathcal{O}(\xi^2(\lambda)) \) as \( n \to \infty \). Substituting this into (4.37), we obtain

\[
\cos \left( \frac{1}{3} \arccos \left( \frac{3q_3}{p_-} \sqrt{-\frac{3}{p_-}} - \frac{2m}{3} \right) \right) = \left\{ \begin{array}{l}
\cos \left( \frac{1-2m}{3} \pi \right) - \sin \left( \frac{1-2m}{3} \pi \right) \mathcal{O}(\Delta^3) \left( 1 - \frac{a}{9} \Delta^2 \right) \\
- \left\{ \frac{\xi(\lambda)}{3} + \mathcal{O}(\xi^3(\lambda)) \right\} \sin \left( \frac{\pi}{3} - \frac{2m}{3} \pi \right) + \mathcal{O}(\Delta^4) \quad \text{as} \quad n \to \infty.
\end{array} \right.
\]

(4.38)

First, we shall show (1.8). Note that \( \lambda = \frac{1}{2} + \frac{1}{12n}, \frac{1}{2} - \frac{1}{12n} \) corresponds to \( m = 2 \). Thus, it follows by (4.38) that

\[
\cos \left( \frac{1}{3} \arccos \left( \frac{3q_3}{2p_-} \sqrt{-\frac{3}{p_-}} - \frac{4m}{3} \frac{\pi}{3} \right) \right) = -1 + \frac{a}{9} \Delta^2 + \mathcal{O}(\Delta^4) \quad \text{as} \quad n \to \infty.
\]

(4.39)

Since there exists some \( \theta_4 \in (0,1) \) such that \( \sqrt{1+x} = 1 + \frac{1}{2} x - \frac{1}{4(1+\theta_4 x)^3} x^2 \) owing to Taylor’s theorem, we have

\[
\sqrt{-\frac{p_-}{3}} = \left( \frac{1}{4} + \frac{\Delta^2}{432} + \mathcal{O}(\Delta^4) \right) \quad \text{as} \quad n \to \infty,
\]

(4.40)

where \( p_- = \frac{3}{16} + \frac{\Delta^2}{16} + \frac{\Delta^2}{243} \). This combined with (4.39) yields

\[
z_{\frac{1}{2} + \frac{1}{12n}} = -\frac{1}{2} + \frac{119}{72} \frac{\Delta^2}{54} \left( \lambda_{\frac{1}{2},p+12n} \right) + \mathcal{O}(\Delta^4) \quad \text{as} \quad n \to \infty
\]

for \( p = 3, 9 \). Using \( \Delta^2 = z + \frac{1}{2} + \frac{\Delta^2}{27} \), we have \( \Delta^2 = \frac{263}{27\cdot72} \Delta^2 + \mathcal{O}(\Delta^4) \) as \( n \to \infty \). Thus, we have

\[
\cos 2\chi(\lambda) = -1 + \frac{263}{27\cdot72} \Delta^2 + \mathcal{O}(\Delta^4) \quad \text{as} \quad n \to \infty,
\]

(4.41)

putting \( \Delta(\lambda) = \cos \chi(\lambda) \). In a similar way to (4.22), we have

\[
\cos 2\chi(\lambda_{\frac{1}{2},3+12n}) = -1 + \frac{1}{2} (e_{\frac{1}{2},3+12n} \pm 2) \left( e_{\frac{1}{2},3+12n} \pm 2 \right)^2 + \mathcal{O}(\left( e_{\frac{1}{2},3+12n} \pm 2 \right)^3) \quad \text{as} \quad n \to \infty,
\]

where

\[
e_{\frac{1}{2},3+12n} = 2 \sqrt{\lambda_{\frac{1}{2},3+12n} - 2n_{\frac{1}{2},3+12n} - \frac{q_0}{u_{\frac{1}{2},3+12n}} + o \left( \frac{1}{n^2} \right)}
\]

as \( n \to \infty \). Comparing this and (4.41), we have

\[
(e_{\frac{1}{2},3+12n})^2 = \frac{263}{27 \times 36} \Delta^2 + \mathcal{O}(\Delta^4) \quad \text{as} \quad n \to \infty.
\]

(4.42)
In a similar way to (4.30), we have
\[
\Delta_-(\lambda) = -\frac{q_{s,0,n,p} + O\left(\frac{1}{\pi}\right)}{2n^\pm_{\lambda,3+12n}} (4.43)
\]
as \(\sqrt{\lambda} = n^\pm_{\lambda,3+12n} + O\left(\frac{1}{\pi}\right)\) and \(n \to \infty\) for \(p = 1,3,5,7,9,11\). Substituting (4.43) into (4.42), we obtain
\[
(\epsilon^\pm_{\lambda,3+12n})^2 = \frac{263(q_{s,0,n,3} + O\left(\frac{1}{n}\right))^2}{27 \times 36 \times 4(n^\pm_{\lambda,3+12n})^2} + O(\Delta^4) \text{ as } n \to \infty.
\]
Since \(\Delta_-(\lambda) = o\left(\frac{1}{\sqrt{\lambda}}\right)\) as \(|\lambda| \to \infty\) and \(\lambda \in \mathbb{R}\), we have
\[
(\epsilon^\pm_{\lambda,3+12n})^2 = \frac{\sqrt{789}}{108n^\pm_{\lambda,3+12n}} \left( (q_{s,0,n,3} + O\left(\frac{1}{n}\right))^2 + O\left(\frac{1}{n^4}\right) \right) \text{ as } n \to \infty.
\]
By the definition of \(\epsilon^\pm_{\lambda,3+12n}\), we have
\[
2\sqrt{\frac{\lambda^\pm_{\lambda,3+12n}}{\lambda}} = -\frac{q_{s,0,n,3}}{u^\pm_{\lambda,3+12n}} + O\left(\frac{1}{n^2}\right) = \pm \frac{\sqrt{789}}{108u^\pm_{\lambda,3+12n}} \left( (q_{s,0,n,3} + O\left(\frac{1}{n}\right))^2 + O\left(\frac{1}{n^4}\right) \right),
\]
which implies (1.8) for \(p = 3\). In a similar way, we obtain (1.8) for \(p = 9\).

In order to show (1.9), we consider \(\lambda^\pm_{\lambda,1+12n}\) as a representative. Namely, we deal with the case where \(m = 1\). It follows by (4.20) and \(\xi(\lambda) = O(\Delta_-)\) as \(\lambda \to +\infty\) that \(\xi^2(\lambda) = 2a\Delta_-^2 + O(\Delta^4)\) as \(\lambda \to +\infty\). Since \(\xi(\lambda) = \arccos(-1 + a\Delta_-^2) - \pi\), we see that \(\xi(\lambda) \leq 0\). Thus, we obtain
\[
\xi(\lambda) = -\sqrt{2a\Delta_-^2 + O(\Delta^4)} = -\sqrt{2a\Delta_-^2 \left[ 1 + O(\Delta_-^2) \right]} = -\sqrt{2a}\Delta_-|\Delta_-| + O(\Delta_-^2) (4.44)
\]
as \(n \to \infty\), due to the existence of some \(\theta \in (0,1)\) satisfying \(\sqrt{1+x} = 1 + \frac{x}{2\sqrt{1+\theta x}}\). On the other hand, (4.38) in the case of \(m = 1\) implies that
\[
\cos \left(\frac{1}{3} \arccos \left(\frac{3q_- - \sqrt{3}}{2p_-} \left[ \frac{3}{p_-} - \frac{2\pi}{3}\right]\right)\right) = \frac{1}{2} + \frac{\xi(\lambda)}{2\sqrt{3}} + O(\Delta_-^2) \text{ as } \lambda \to +\infty,
\]
using \(\xi(\lambda) = O(\Delta_-)\). This together with (4.17), (4.40) and (4.44) yields
\[
z^\pm_{1,\lambda} = \frac{1}{4} - \frac{a}{2\sqrt{3}}|\Delta_-| + O(\Delta_-^2)
and hence
\[ \Delta^2(\lambda^+_{N,1+12n}) = z + \frac{1}{2} + \frac{\Delta^2}{27} - \frac{3}{4} - \frac{a}{2\sqrt{3}} \left| \Delta_- (\lambda^+_{N,1+12n}) \right| + O(\Delta^2 (\lambda^+_{N,1+12n})) \text{ as } n \to \infty. \]

Putting \( \Delta(\lambda) = \cos \chi(\lambda) \), we obtain
\[ \cos 2\chi(\lambda) = \frac{1}{2} - \frac{a}{\sqrt{3}} \left| \Delta_- (\lambda^+_{N,1+12n}) \right| + O(\Delta^2 (\lambda^+_{N,1+12n})) \text{ as } n \to \infty. \quad (4.45) \]

We put
\[ e^+_{N,1+12n} = 2\sqrt{\lambda^+_{N,1+12n}} - 2u^+_{N,1+12n} - \frac{q_0}{u^+_{N,1+12n}} + o \left( \frac{1}{n^2} \right) \]
as \( n \to \infty \). Then, we have
\[ \cos \chi(\lambda^+_{N,1+12n}) = \cos \left( 2u^+_{N,1+12n} + e^+_{N,1+12n} \right) = \cos 2u^+_{N,1+12n} - \left( \sin 2u^+_{N,1+12n} \right) e^+_{N,1+12n} + O((e^+_{N,1+12n})^2) = \frac{1}{2} - \frac{\sqrt{3}}{2} e^+_{N,1+12n} + O((e^+_{N,1+12n})^2) \quad (4.46) \]
as \( n \to \infty \). Comparing (4.45) and (4.46), we have \( e^+_{N,1+12n} \geq 0 \) and
\[ (e^+_{N,1+12n})^2 = \frac{4}{9} a^2 \Delta^2_- + O(\Delta^3 (\lambda^+_{N,1+12n})) \quad \text{as } n \to \infty. \quad (4.47) \]

Substituting (4.43) and \( \Delta_- (\lambda) = o \left( \frac{1}{\sqrt{\lambda}} \right) \) as \( |\lambda| \to \infty \) into this, we have
\[ (e^+_{N,1+12n})^2 = \frac{a^2}{9} \left( \frac{q_{s,0,n,1} + O \left( \frac{1}{n} \right)}{(u^+_{N,1+12n})^2} \right)^2 + o \left( \frac{1}{n^3} \right) \]
as \( n \to \infty \). Taking (4.47) into account, we have
\[ 2\sqrt{\lambda^+_{N,1+12n}} = 2u^+_{N,1+12n} + \frac{q_0}{u^+_{N,1+12n}} + o \left( \frac{1}{n^2} \right) + \sqrt{\frac{a^2}{9} \left( \frac{q_{s,0,n,1} + O \left( \frac{1}{n} \right)}{(u^+_{N,1+12n})^2} \right)^2 + o \left( \frac{1}{n^3} \right)} \]
as \( n \to \infty \). Thus, we obtain
\[ 4\lambda^+_{N,1+12n} = 4(u^+_{N,1+12n})^2 + 4q_0 + o \left( \frac{1}{n} \right) + 4 \sqrt{\frac{a^2}{9} q_{s,0,n,1} + o \left( \frac{1}{n} \right)} \]
as \( n \to \infty \). This yields (1.9) for \( \lambda^+_{N,1+12n} \). In a similar way, we obtain (1.9) for \( \lambda^-_{N,1+12n} \) and \( \lambda^\pm_{N,p+12n} \) in the case where \( p = 5, 7, 11 \).

\[ \square \]

**Proof of Theorem 1.4.** If \( \Delta(\lambda) = 0 \) and \( q \) is even, (3.1) yields \( D(\frac{N}{2}, \lambda) = 0 \). This implies \( \gamma_{\frac{N}{2},12n-9} = \gamma_{\frac{N}{2},12n-3} = \emptyset \). Moreover, Lemmas 4.3 and 4.5 imply the desired statements except for this.

\[ \square \]
5 Further comments

Throughout this paper, we dealt with a class of zigzag supergraphene-based carbon nanotubes by adding extra number of carbon atoms on the standard zigzag carbon nanotubes. Our analysis yields results of spectral structure. Especially, by using the standard method established Floquet and Bloch, we obtained the dispersion relation and the spectral discriminant (see (1.2), which is the polynomial of the discriminant $\Delta(\lambda)$ of the corresponding Hill operator with the 6 degree and without the part of odd degree. This fact is suited to Viète’s method for a class of cubic equations. In the case of standard zigzag carbon nanotube [10], it turns out that $F_0(\lambda) = 2\Delta^2(\lambda) + \frac{\theta'(1,\lambda)\varphi(1,\lambda)}{4} - 1$ plays roles of the spectral discriminant. In the case where there are no carbon atoms on each edge, the spectral discriminant is the polynomial of $\Delta(\lambda)$ with 2 degree and without the part of odd degree. Although we add two carbon atoms for each edge in this paper, there are of course an interest in the case of the zigzag carbon nanotubes with extra carbon atoms for any $n \in \mathbb{N}$. For such a model, we predict that its spectral discriminant can be the polynomial of $\Delta(\lambda)$ with $2n$ degree and no odd degree. If this conjecture is true, then its explicit analysis of the spectrum could be possible for only the case where $n = 0, 1, 2, 3, 4$ because there is no algebraic formula for the roots of the algebraic equations with the degree $n \geq 5$. In this sense, this paper is rather approaching the limit of the explicit spectral analysis of zigzag carbon nanotube with extra carbon atoms.

Next, we leave a comment on the relationship between the flat band of $\sigma(H)$ and the one in [10]. In our paper, we add two extra carbon atoms on each edge, but we imposed the Kirchhoff vertex condition at each vertex for the simplicity. Since the Kirchhoff vertex condition consists of the continuity of wave functions and no flux conditions, one is interested in the relationship between the flat band of $H$ and the Hamiltonian in [10]. Let $K$ be the Hamiltonian of [10] (Note that $\sigma(K) = \sigma_D(L)$ and $\sigma(H) = \sigma_D(L) \cup \sigma_2(L) \cup \sigma_{-\frac{3}{2}}(L)$). Let $Q(x) = q(\{x\})$ for $x \in (0, 3)$, where $\{x\}$ stands for the fractional part of $x$. We put $L_1 = -\frac{d^2}{dx^2} + Q(x)$ in $L^2(0, 1)$ and $L_3 = -\frac{d^2}{dx^2} + Q(x)$ in $L^2(0, 3)$. Then, we have the following:

Lemma 5.1. We have $\sigma_D(L_3) = \sigma_D(L_1) \cup \sigma_2(L_1) \cup \sigma_{-\frac{3}{2}}(L_1)$.

Proof. Recall $\theta(x, \lambda)$ and $\varphi(x, \lambda)$ be the fundamental solutions to $L_1$. Then, we notice that $\lambda \in \sigma_D(L_3)$ if and only if $\varphi_3(3, \lambda) = 0$. Using the monodromy matrix

$$M(\lambda) = \begin{pmatrix} \theta(1, \lambda) & \varphi(1, \lambda) \\ \theta'(1, \lambda) & \varphi'(1, \lambda) \end{pmatrix},$$

we obtain

$$\begin{pmatrix} \theta(3, \lambda) & \varphi(3, \lambda) \\ \theta'(3, \lambda) & \varphi'(3, \lambda) \end{pmatrix} = M^3(\lambda).$$

This yields $\varphi(3, \lambda) = \varphi_1\left(\theta_3^2 + \theta_1'\varphi_1 + \theta_1\varphi_1' + (\varphi_1')^2\right)$. Using $\Delta = \frac{\theta_1 + \varphi_1'}{2}$ and $\theta_1\varphi_1' - \theta_1'\varphi_1 = 1$, we obtain $\varphi(3, \lambda) = \varphi_3(\lambda)(2\Delta(\lambda) - 1)(2\Delta(\lambda) + 1)$. This implies our claim in this lemma. \qed
In this sense, our model can be considered as a special case of [10] under the additional assumption $Q(x) = q(x)$. In this case, we found a fact due to the strength of carbine-like chain in the sense of Theorem 1.4. According to Theorem 1.4(i), even if any potential $q \in L^2(0,1)$ is given, then the $(12n-10)$ and $(12n-9)$th spectral bands never be separate, namely, $\gamma_{0,12n-10} = \emptyset$. In the case of $K$, we can find the possibility of absent even-numbered spectral gap in Theorem 3.3 in [10]. In our special case, we gave a deeper result for the band structure, especially the strength of the connection of spectral bands. As for the classical Hill operator, the existence of absent spectral gap is a rather subtle problem: If we give a very small perturbation for the Hill operator with absent spectral gaps, then the absence of spectral gaps is easy to collapse. In this sense, we find that Theorem 1.4 (i) states the strength of carbine-like chains.

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