12, October, 2015

Schrödinger operators on a periodically broken zigzag carbon nanotube

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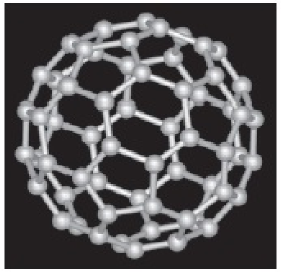
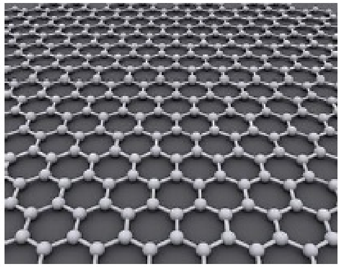
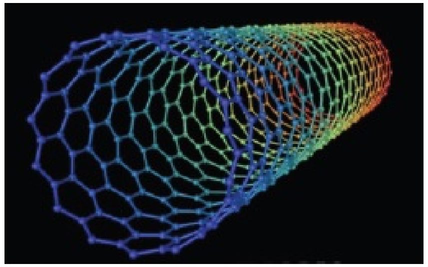
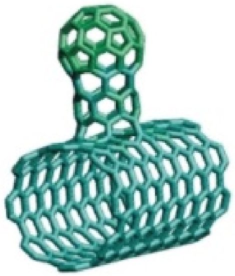
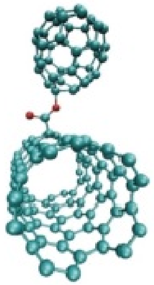
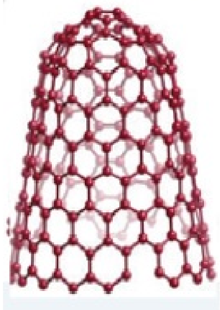
1 Introduction

A Family of Allotropes of Carbon[*1]

※ Fullerenes, Graphene, Carbon nanotube, Carbon nanobud, Carbon nanohorn, Graphyne, Carbon nanofoam...

[*1] http://www.nec.com/, http://ja.wikipedia.org/wiki/

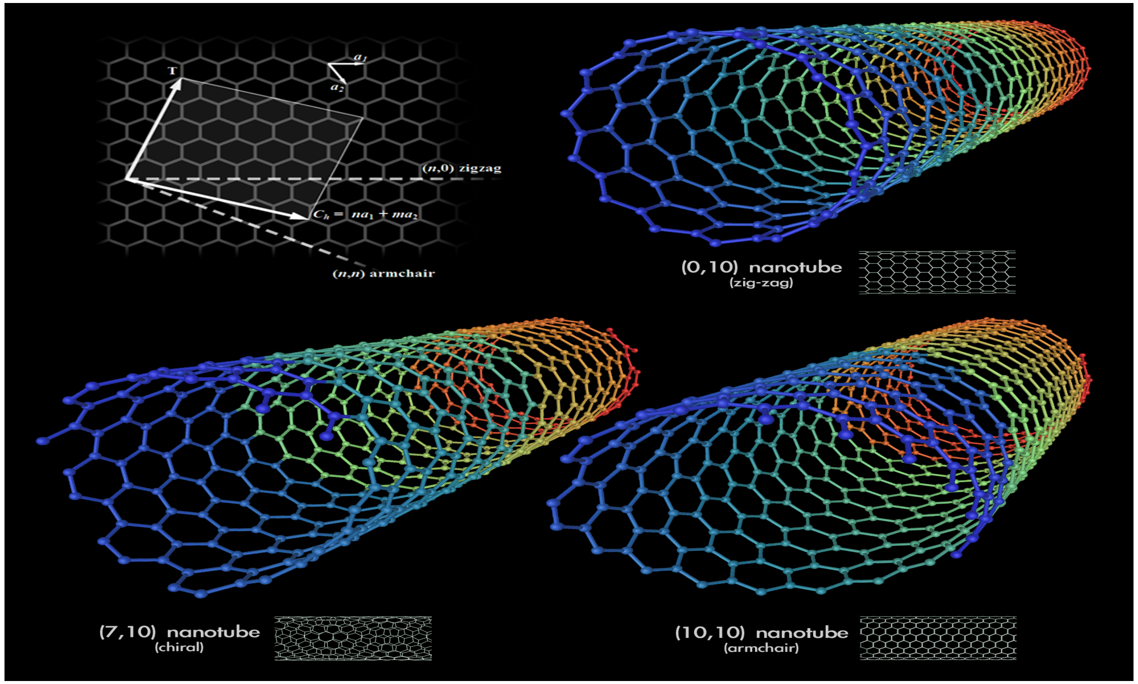


Fig. 1 Zigzag, Armchair and Chiral Nanotube. © wikipedia.

Quantum graph approach for carbon nanotubes:

- Kuchment and Post(2007)
- Korotyaev and Lobanov(2007)

In this study, we consider spectra on a broken carbon nanotube.

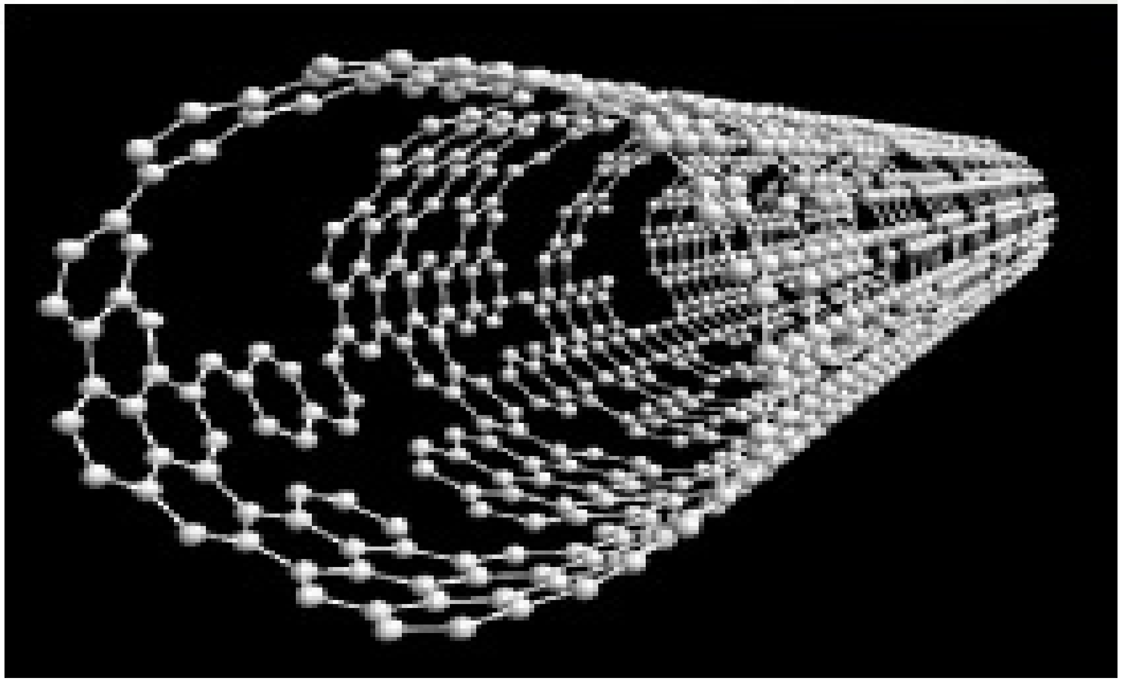


Fig. 2 A broken carbon nanotube. © Akira Koshio.

Broken Carbon Nanotube

In a process to refine single wall carbon nanotubes, we need metals such as Ni, Co, Y and Fe. So, carbon nanotubes are strained with tiny particles of metals. In order to get rid of these metals, we need to clean by acids. Carbon nanotubes are broken in these process.

cf: There are a method to refine single wall carbon nanotubes without any metal.
(metal-free thermal CVD , Akira Koshio, 2011)

In this study, we get rid of edges from a metric graph corresponding to the zigzag carbon nanotubes and call them broken zigzag carbon nanotubes.

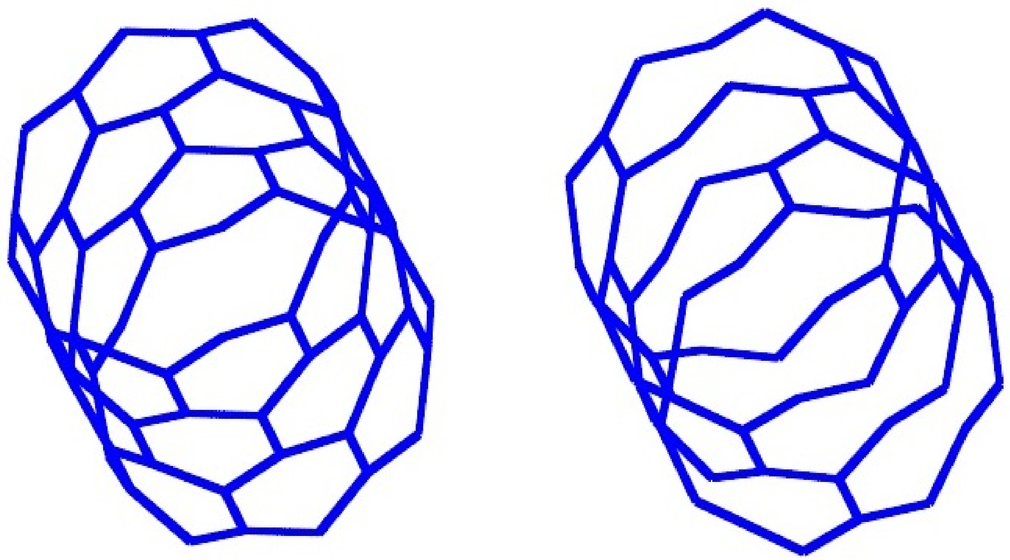


Fig. 3 A pure zigzag carbon nanotube (Left) and a broken zigzag carbon nanotube (Right).

Throughout this talk, we consider only the zigzag carbon nanotubes:

Definition 1.1 (A pure zigzag carbon nanotube)**.**
For a fixed number $N \in \mathbb{N}$*, we call*

$$\tilde{\Gamma}^N = \bigcup_{\omega=(n,j,k)\in\tilde{\mathcal{Z}}} \tilde{\Gamma}_\omega$$

the zigzag carbon nanotube with N*-zigzag, where* $\tilde{\mathbb{J}} = \{0, 1, 2\}$, $\mathbb{Z}_N = \mathbb{Z}/(N\mathbb{Z})$, $\tilde{\mathcal{Z}} := \mathbb{Z} \times \tilde{\mathbb{J}} \times \mathbb{Z}_N$ *and* $\tilde{\Gamma}_\omega (\simeq [0, 1])$ *be an edge in Fig. 2 for* $\omega \in \tilde{\mathcal{Z}}$*.*

Before we see the precise definition of $\tilde{\Gamma}_\omega$, let us see its picture:

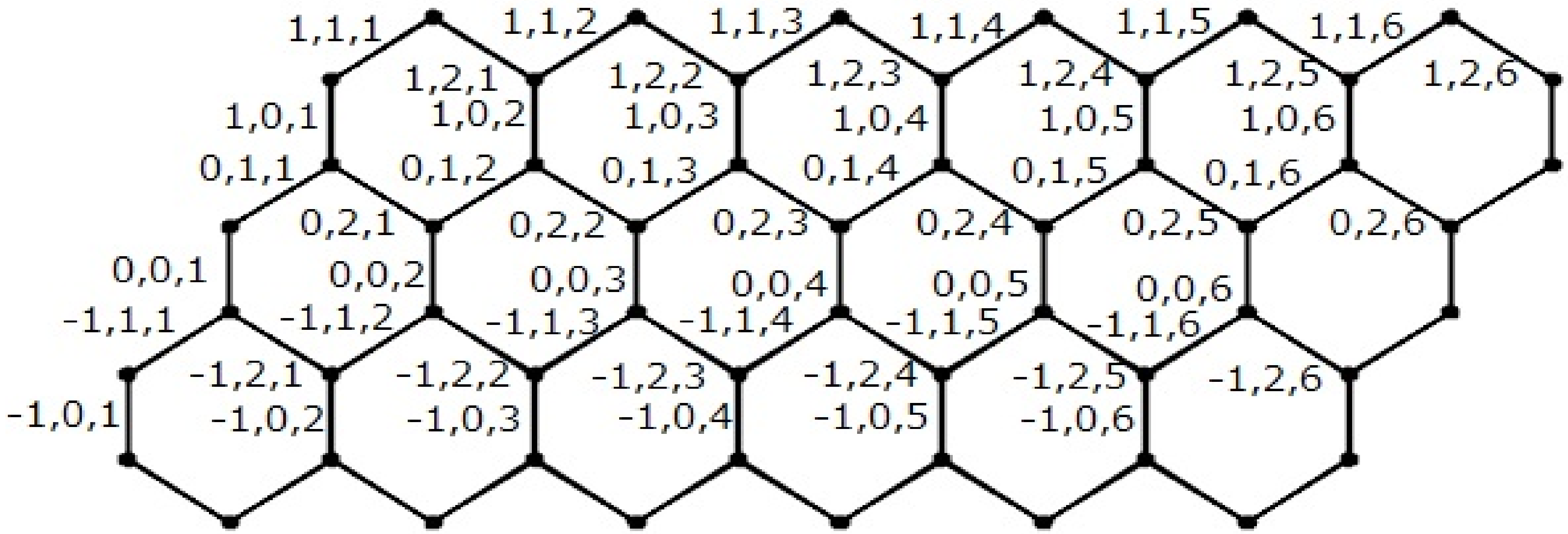


Fig. 4 Cutting and opening $\tilde{\Gamma}^6$, we obtain the above lattice. The indexes imply the ones of $\tilde{\Gamma}_{n,j,k}$.

Definition 1.2 (The precise definition of each edge $\tilde{\Gamma}_{n,j,k}$).

Let $R_N = \frac{\sqrt{3}}{4\sin\frac{\pi}{2N}}$. *For* $\omega = (n, j, k) \in \tilde{\mathcal{Z}}$, *we define* $\tilde{\Gamma}_\omega = \{\mathbf{x} = \mathbf{r}_\omega + t\mathbf{e}_\omega | \quad 0 \leq t \leq 1\} (\simeq [0, 1])$, *where*

$$
\begin{aligned}
&c_k = \cos\frac{\pi k}{N}, \quad s_k = \sin\frac{\pi k}{N}, \quad \kappa_k = R_N(c_k, s_k, 0),\\
&\mathbf{e}_{n,0,k} = (0, 0, 1), \quad \mathbf{e}_0 = (0, 0, 1),\\
&\mathbf{e}_{n,1,k} = \kappa_{n+2k+1} - \kappa_{n+2k} + \frac{\mathbf{e_0}}{2},\\
&\mathbf{e}_{n,2,k} = \kappa_{n+2k+2} - \kappa_{n+2k+1} - \frac{\mathbf{e}_0}{2},\\
&\mathbf{r}_{n,0,k} = \kappa_{n+2k} + \frac{3n}{2}\mathbf{e}_0,\\
&\mathbf{r}_{n,1,k} = \mathbf{r}_{n,0,k} + \mathbf{e}_0, \quad \mathbf{r}_{n,2,k} = \mathbf{r}_{n+1,0,k}.
\end{aligned}
$$

We now get rid of some of vertical edges from $\tilde{\Gamma}^{2N}$ for a fixed $N \in \mathbb{N}$.

Definition 1.3 (A broken zigzag carbon nanotube). *Let* $\mathcal{Z} := \mathbb{Z} \times \mathbb{J} \times \mathbb{Z}_N$, *where* $\mathbb{J} := \{1, 2, 3, 4, 5\}$. *For* $(n, j, k) \in \mathcal{Z}$, *we consider edges* $\Gamma_{n,j,k}$ *defined as follows:* $\Gamma_{n,1,k} = \tilde{\Gamma}_{n,0,2k-1}$, $\Gamma_{n,2,k} = \tilde{\Gamma}_{n,1,2k-1}$, $\Gamma_{n,3,k} = \tilde{\Gamma}_{n,2,2k-1}$, $\Gamma_{n,4,k} = \tilde{\Gamma}_{n,1,2k}$ *and* $\Gamma_{n,5,k} = \tilde{\Gamma}_{n,2,2k}$. *We call*

$$\Gamma^N = \bigcup_{\omega \in \mathcal{Z}} \Gamma_\omega$$

a broken zigzag carbon nanotube[*2].

[*2] The right picture in Fig. 3 is the one in the case of $N = 4$.

Cutting and opening Γ^3, we obtain the lattice in Fig. 5. The indexes in this picture imply the ones of $\Gamma_{n,j,k}$.

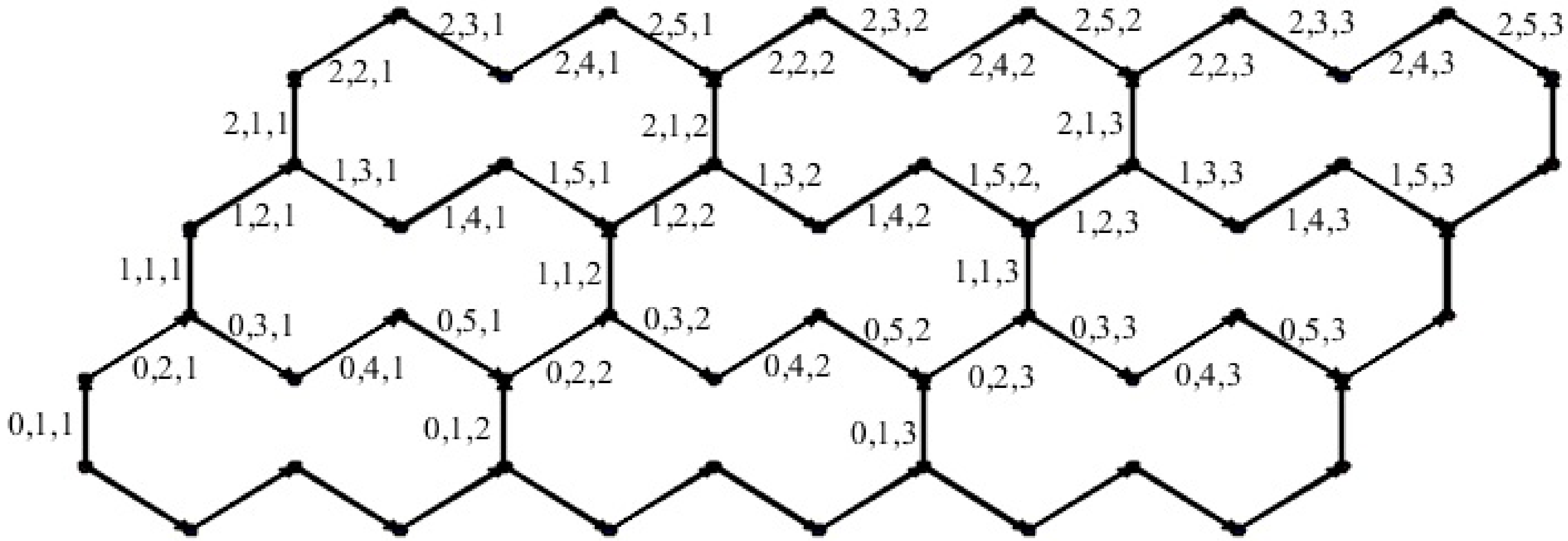


Fig. 5 A broken zigzag carbon nanotube Γ^3.

Let us define periodic Schrödinger operators in the Hilbert space $\mathcal{H} := L^2(\Gamma^N) = \oplus_{\omega \in \mathcal{Z}} L^2(\Gamma_\omega)$, where $L^2(\Gamma_\omega) := L^2([0,1])$. For a real-valued function $q \in L^2(0,1)$, we define

$$(Hf_\omega)(x) = -f_\omega''(x) + q(x) f_\omega(x), \quad x \in (0,1) \simeq \Gamma_\omega^\circ, \quad \omega \in \mathcal{Z},$$

$$\mathrm{Dom}(H) = \left\{ \bigoplus_{\omega \in \mathcal{Z}} f_\omega \in L^2(\Gamma^N) \;\middle|\; \begin{array}{c} \bigoplus_{\omega \in \mathcal{Z}} (-f_\omega'' + q f_\omega) \in L^2(\Gamma^N), \\ -f_{n,1,k}'(1) + f_{n,2,k}'(0) - f_{n,5,k-1}'(1) = 0, \\ f_{n,1,k}(1) = f_{n,2,k}(0) = f_{n,5,k-1}(1), \\ -f_{n,2,k}'(1) + f_{n,3,k}'(0) + f_{n+1,1,k}'(0) = 0, \\ f_{n,2,k}(1) = f_{n,3,k}(0) = f_{n+1,1,k}(0), \\ f_{n,3,k}(1) = f_{n,4,k}(0), \; f_{n,3,k}'(1) = f_{n,4,k}'(0), \\ f_{n,4,k}(1) = f_{n,5,k}(0), \; f_{n,4,k}'(1) = f_{n,5,k}'(0) \\ \text{for} \quad n \in \mathbb{Z} \text{ and } k \in \mathbb{Z}_N \end{array} \right\}.$$

Definition 1.4 (A degenerate broken zigzag nanotube).
We call Γ^1 *a degenerate broken zigzag nanotube.*

For convenience, we put $\Gamma_{n,j} = \Gamma_{n,j,1}$ for $n \in \mathbb{Z}$ and $j \in \mathbb{J}$. Then, we have the flag-like metric graph in Fig. 6.

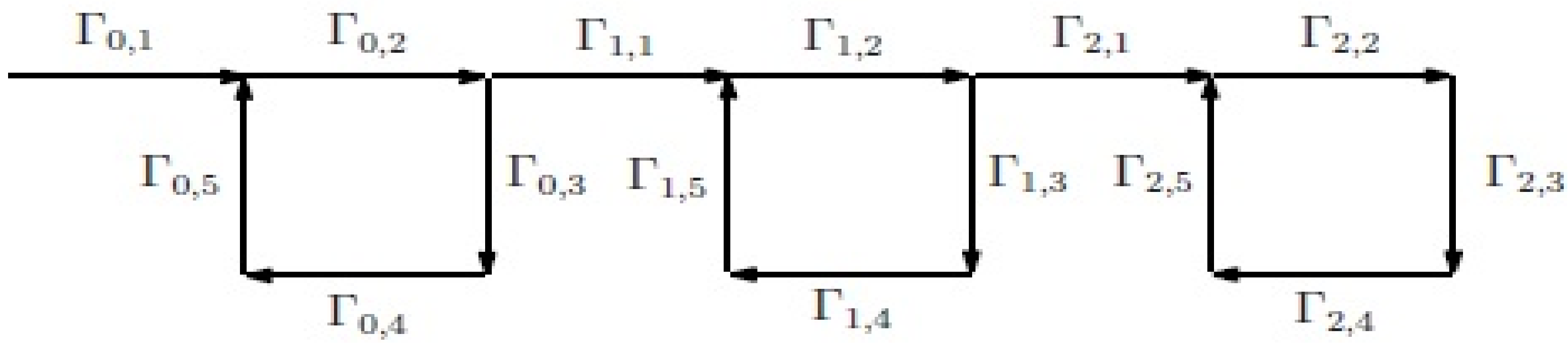


Fig. 6 A degenerate broken zigzag nanotube Γ^1.

Let $\mathcal{Z}_1 := \mathbb{Z} \times \mathbb{J}$. We fix $N \in \mathbb{N}$ and put $s = e^{i\frac{2\pi}{N}}$. For $k = 1, 2, \ldots, N$, we define H_k in $L^2(\Gamma^1)$ as follows:

$$(H_k f_{n,j})(x) = -u''_{n,j}(x) + q(x)u_{n,j}(x),\ x \in (0,1) \simeq \Gamma^\circ_{n,j},\ (n,j) \in \mathcal{Z}_1,$$

$$\mathrm{Dom}(H_k)$$

$$= \left\{ \bigoplus_{(n,j)\in\mathcal{Z}_1} u_{n,j} \in L^2(\Gamma^1) \;\middle|\; \begin{array}{c} \bigoplus_{(n,j)\in\mathcal{Z}_1}(-u''_{n,j} + qu_{n,j}) \in L^2(\Gamma^1), \\ -u'_{n,1}(1) + u'_{n,2}(0) - s^k u'_{n,5}(1) = 0, \\ u_{n,1}(1) = u_{n,2}(0) = s^k u_{n,5}(1), \\ -u'_{n,2}(1) + u'_{n,3}(0) + u'_{n+1,1}(0) = 0, \\ u_{n,2}(1) = u_{n,3}(0) = u_{n+1,1}(0), \\ u_{n,3}(1) = u_{n,4}(0),\ u'_{n,3}(1) = u'_{n,4}(0), \\ u_{n,4}(1) = u_{n,5}(0),\ u'_{n,4}(1) = u'_{n,5}(0) \\ \text{for} \quad n \in \mathbb{Z} \end{array} \right\}.$$

- Utilizing the same method as [Korotyaev and Lobanov, '07], we obtain a unitary operator satisfying the following unitarily equivalence:

$$H \simeq \oplus_{k=1}^{N} H_k.$$

<u>On the unitary equivalence of H and $\bigoplus_{k=1}^{N} H_k$</u>

For $f \in L^2(\Gamma^N)$, we identify f as the sequence of vectors as follows:

$$f = (f_{n,j,k})_{(n,j,k)\in\mathcal{Z}} = (f_{n,j})_{(n,j)\in\mathcal{Z}_1} = (\begin{pmatrix} f_{n,j,1} \\ f_{n,j,2} \\ \vdots \\ f_{n,j,N} \end{pmatrix})_{(n,j)\in\mathcal{Z}_1}.$$

Then, the operator H can be written as follows:

$$(Hf_{n,j})(x) = \begin{pmatrix} -f''_{n,j,1}(x) + q(x)f_{n,j,1}(x) \\ -f''_{n,j,2}(x) + q(x)f_{n,j,2}(x) \\ \vdots \\ -f''_{n,j,N}(x) + q(x)f_{n,j,N}(x) \end{pmatrix}, \quad (n,j) \in \mathcal{Z}_1,$$

$$\begin{aligned} &\mathrm{Dom}(H) \\ &= \left\{ \bigoplus_{\alpha \in \mathcal{Z}_1} f_\alpha \in L^2(\Gamma^N) \;\middle|\; \begin{array}{l} \bigoplus_{\alpha \in \mathcal{Z}_1} (-f''_\alpha + qf_\alpha) \in L^2(\Gamma^N), \\ -f'_{n,1}(1) + f'_{n,2}(0) - Sf'_{n,5}(1) = 0, \\ f_{n,1}(1) = f_{n,2}(0) = Sf_{n,5}(1), \\ f'_{n+1,1}(0) - f'_{n,2}(1) + f'_{n,3}(0) = 0, \\ f_{n+1,1}(0) = f_{n,2}(1) = f_{n,3}(0), \\ f_{n,3}(1) = f_{n,4}(0), \quad f'_{n,3}(1) = f'_{n,4}(0), \\ f_{n,4}(1) = f_{n,5}(0), \quad f'_{n,4}(1) = f'_{n,5}(0) \\ \text{for} \quad n \in \mathbb{Z} \end{array} \right\}. \end{aligned}$$

Here, S is the following matrix:

$$S = \begin{pmatrix} 0 & 0 & 0 & \cdots & 0 & 1 \\ 1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 1 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1 & 0 \end{pmatrix}.$$

The eigenvalues of the matrix S are $\{s^k\}_{k=1}^N$, where $s = e^{i\frac{2\pi}{N}}$. For each k, the eigenvector corresponding to s^k is

$$v_k = \frac{1}{\sqrt{N}}\ {}^t(1, s^{-k}, s^{-2k}, \cdots, s^{-(N-1)k}).$$

The matrix S can be decomposed as

$$S = s\mathcal{P}_1 + s^2\mathcal{P}_2 + \cdots + s^N\mathcal{P}_N,$$

by using the matrices $\mathcal{P}_1, \mathcal{P}_2, \ldots, \mathcal{P}_N$ satisfying

$$\mathcal{P}_k u = (u, v_k) v_k \qquad (u \in \mathbf{C}^N) \quad \text{and} \quad I = \mathcal{P}_1 + \cdots + \mathcal{P}_N.$$

Thus, for any $f = \left(\begin{pmatrix} f_{n,j,1} \\ f_{n,j,2} \\ \vdots \\ f_{n,j,N} \end{pmatrix} \right)_{(n,j)\in\mathcal{Z}_1} \in L^2(\Gamma^N)$, we have

$$\begin{pmatrix} f_{n,j,1} \\ f_{n,j,2} \\ \vdots \\ f_{n,j,N} \end{pmatrix} = \mathcal{P}_1 \begin{pmatrix} f_{n,j,1} \\ f_{n,j,2} \\ \vdots \\ f_{n,j,N} \end{pmatrix} + \cdots + \mathcal{P}_N \begin{pmatrix} f_{n,j,1} \\ f_{n,j,2} \\ \vdots \\ f_{n,j,N} \end{pmatrix}$$

$$= (f_{n,j}, v_1) v_1 + \cdots + (f_{n,j}, v_N) v_N$$

Considering the unitary operator $U : L^2(\Gamma^N) \to \oplus_{k=1}^N L^2(\Gamma^1)$

$$Uf = ((f_\alpha, v_1)_{\alpha\in\mathcal{Z}_1}, \dots, (f_\alpha, v_N)_{\alpha\in\mathcal{Z}_1}), \quad f = (\begin{pmatrix} f_{\alpha,1} \\ f_{\alpha,2} \\ \vdots \\ f_{\alpha,N} \end{pmatrix})_{\alpha\in\mathcal{Z}_1},$$

we have

$$UHU^{-1} = \oplus_{k=1}^N H_k.$$

- Thus, it is sufficient to examine $\sigma(H_k)$ in order to examine $\sigma(H)$.
- In order to examine $\sigma(H_k)$, we recall the spectral theory for the corresponding Hill operator $L := -d^2/dx^2 + q$ in $L^2(\mathbb{R})$, where the real valued function $q \in L^2(0,1)$, appearing as the potential of H, is extended to the 1-periodic function on $\mathbb{R}$.

Spectral Theory for the Hill operator

For $\lambda \in \mathbb{C}$, let $\theta(x, \lambda)$ and $\varphi(x, \lambda)$ be the solutions to the Schrödinger equation

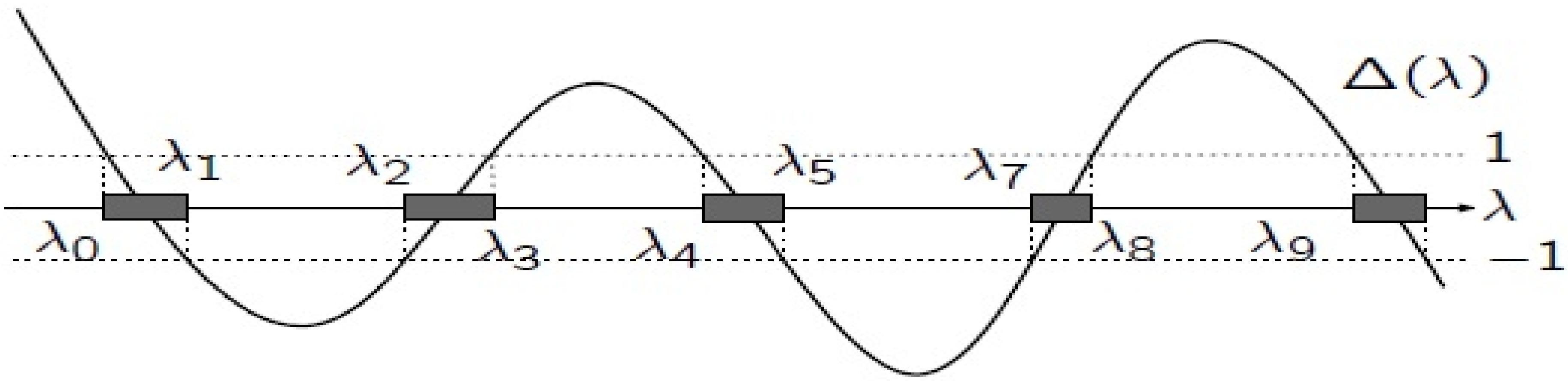
$$-y''(x, \lambda) + q(x)y(x, \lambda) = \lambda y(x, \lambda), \quad x \in \mathbb{R}, \tag{1}$$

as well as the initial conditions $\theta(0, \lambda) = 1$, $\theta'(0, \lambda) = 0$ and $\varphi(0, \lambda) = 0$, $\varphi'(0, \lambda) = 1$, respectively.

(I) 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 $\lambda \in \mathbb{C}$.



(II) It is known as the Floquet–Bloch theory that the spectrum of L is characterized by $\Delta(\lambda)$ as

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

where $\lambda_0, \lambda_1, \lambda_2, \ldots$ are zeroes of $\Delta(\lambda) \pm 1$ and are labeled in increasing order.

(III) The zeroes of $\Delta(\lambda) \pm 1$ satisfy the inequality

$$\lambda_0 < \lambda_1 \leq \lambda_2 < \lambda_3 \leq \lambda_4 < \dots .$$

(IV) For $j \in \mathbb{N}$, the interval $B_j := [\lambda_{2j-2}, \lambda_{2j-1}]$ is called the jth 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 called the jth gap of $\sigma(L)$.

(V) 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 $\sigma_D(L) = \{\lambda \in \mathbb{R} | \quad \varphi(1, \lambda) = 0\}$ and $\mu_n \in [\lambda_{2n-1}, \lambda_{2n}]$ for each $n \in \mathbb{N}$.

2 Main Result

Definition 2.1 (The discriminant (Lyapunov function) for $\sigma(H_k)$**).** *For* $\lambda \in \mathbb{C}$*, we define*

$$\Delta^2(\lambda)D(\lambda) = 4\Delta^4(\lambda) + \frac{\theta_1(\lambda)\varphi_1'(\lambda) - 7}{2}\Delta^2(\lambda) + \frac{1 - \theta_1(\lambda)\varphi_1'(\lambda)}{8}, \tag{2}$$

where $\theta_1(\lambda) = \theta(1, \lambda)$ *and* $\varphi_1'(\lambda) = \varphi'(1, \lambda)$*.*
For $k = 1, 2, \ldots, N$*, we define*

$$D(k, \lambda) = \frac{2\Delta^2(\lambda)D(\lambda) + s_k^2}{\sqrt{4\Delta^4(\lambda) - 4\Delta^2(\lambda)s_k^2 + s_k^2}} \tag{3}$$

on $\mathbb{C} \setminus \mathcal{P}_k$*, where*
$\mathcal{P}_k = \{\lambda \in \mathbb{C} | \quad 4\Delta^4(\lambda) - 4\Delta^2(\lambda)s_k^2 + s_k^2 = 0\}$*. Here, we recall* $s_k = \sin\frac{\pi k}{N}$*. We call* $D(k, \lambda)$ *the discriminant for* H_k*.*

Definition 2.2. *For $k = 1, 2, \ldots, N$, let $\sigma_\infty(H_k)$ be the flat band of H_k, namely, the set of all eigenvalues of H_k with infinite multiplicities.*

Utilizing a direct integral decomposition for H_k, we see that the function $D(k, \lambda)$ plays the role of the discriminant for the operator H_k for each $k = 1, 2, \ldots, N$:

Theorem 2.3. *For $k = 1, 2, \ldots, N$, we have $\sigma(H_k) = \sigma_\infty(H_k) \cup \sigma_{ac}(H_k)$, where*

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

For convenience, we put $D(0, \lambda) = D(N, \lambda)$ and $H_0 = H_N$. Since $s_{N-k} = \sin \frac{\pi(N-k)}{N} = \sin \frac{\pi k}{N} = s_k$ for $k = 1, 2, \ldots, N$, we have $D(k, \lambda) = D(N - k, \lambda)$ for $k = 1, 2, \ldots, N$.

Thus, it is sufficient to examine the properties of the discriminants

$$D(0, \lambda), D(1, \lambda), \ldots, D(\ell - 1, \lambda)$$

if $N = 2\ell - 1$ and $\ell \in \mathbb{N}$. On the other hand, it is sufficient to examine the properties of the discriminants

$$D(0, \lambda), D(1, \lambda), \ldots, D(\ell - 1, \lambda), D(\ell, \lambda)$$

if $N = 2\ell$ and $\ell \in \mathbb{N}$.
Let $\ell_N = [\frac{N-1}{2}]$, where $[x]$ implies the maximal natural number which does not exceed $x \in \mathbb{R}$. Note that $\ell_N = \ell - 1$ in the both case where $N = 2\ell - 1$ and $N = 2\ell$ for a fixed $\ell \in \mathbb{N}$.

Theorem 2.4. *We have the followings:*
(i) For $k = 1, 2, \ldots, N$*, we have* $\sigma_{ac}(H_k) = \sigma_{ac}(H_{N-k})$*.*
(ii) We have $\sigma_{ac}(H) = \cup_{k=0}^{\ell_N} \sigma_{ac}(H_k)$ *if* N *is odd,*
$\sigma_{ac}(H) = \cup_{k=0}^{\ell_N+1} \sigma_{ac}(H_k)$ *otherwise.*
(iii) For $k = 0, 1, 2, \ldots, N$*, there exists real sequence*

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

such that $\sigma_{ac}(H_k) = \bigcup_{j=1}^{\infty} [\lambda_{k,j-1}^{+}, \lambda_{k,j}^{-}]$*.*
(iv) We have the following inequality:

$$\begin{aligned} \lambda_{0,0}^{+} &< \lambda_{0,1}^{-} < \lambda_{0,1}^{+} < \lambda_{0,2}^{-} < \lambda_{0,2}^{+} < \lambda_{0,3}^{-} < \lambda_{0,3}^{+} < \lambda_{0,4}^{-} \leq \lambda_{0,4}^{+} \\ &< \lambda_{0,5}^{-} < \lambda_{0,5}^{+} < \lambda_{0,6}^{-} < \lambda_{0,6}^{+} < \lambda_{0,7}^{-} < \lambda_{0,7}^{+} < \lambda_{0,8}^{-} \leq \lambda_{0,8}^{+} < \cdots \\ &< \lambda_{0,4n-3}^{-} < \lambda_{0,4n-3}^{+} < \lambda_{0,4n-2}^{-} < \lambda_{0,4n-2}^{+} \\ &\qquad < \lambda_{0,4n-1}^{-} < \lambda_{0,4n-1}^{+} < \lambda_{0,4n}^{-} \leq \lambda_{0,4n}^{+} < \cdots . \end{aligned}$$

(v) For $k = 1, 2, \ldots, \ell_N$, we have

$$\lambda^+_{k,0} < \lambda^-_{k,1} \le \lambda^+_{k,1} < \lambda^-_{k,2} \le \lambda^+_{k,2} < \lambda^-_{k,3} \le \lambda^+_{k,3} < \lambda^-_{k,4} < \lambda^+_{k,4}$$
$$< \lambda^-_{k,5} \le \lambda^+_{k,5} < \lambda^-_{k,6} \le \lambda^+_{k,6} < \lambda^-_{k,7} \le \lambda^+_{k,7} < \lambda^-_{k,8} < \lambda^+_{k,8} < \cdots$$
$$< \lambda^-_{k,4n-3} \le \lambda^+_{k,4n-3} < \lambda^-_{k,4n-2} \le \lambda^+_{k,4n-2}$$
$$< \lambda^-_{k,4n-1} \le \lambda^+_{k,4n-1} < \lambda^-_{k,4n} < \lambda^+_{k,4n} < \cdots .$$

- If $s_k \neq \sqrt{\frac{7}{8}}$, then we have $\lambda^-_{k,2n-1} \neq \lambda^+_{k,2n-1}$ for $n \in \mathbb{N}$ and $k = 1, 2, \ldots, \ell_N$. If $q \equiv 0$ and $s_k = \sqrt{\frac{7}{8}}$, then we have $\lambda^-_{k,2n-1} = \lambda^+_{k,2n-1}$ for $n \in \mathbb{N}$ and $k = 1, 2, \ldots, \ell_N$.
- If $k \neq \frac{N}{6}$, then we have $\lambda^-_{k,4n-2} \neq \lambda^+_{k,4n-2}$ for any $k = 1, 2, \ldots, \ell_N$. If $q \equiv 0$ and $k = \frac{N}{6}$, then we have $\lambda^-_{k,4n-2} = \lambda^+_{k,4n-2}$ for any $n \in \mathbb{N}$ and $k = 1, 2, \ldots, \ell_N$.

(vi) Assume that $N = 2\ell$. *Then, we have* $\lambda^-_{\ell,n} < \lambda^+_{\ell,n}$ *for all* $n \in \mathbb{N}$.

(vii) Let $\{\eta_n\}_{n=1}^{\infty} = \{\lambda \in \mathbb{R} | \quad \Delta(\lambda) = 0\}$, $\{\mu_n\}_{n=1}^{\infty} = \sigma_D(L)$ *and* $\{\xi_n\}_{n=1}^{\infty} = \{\lambda \in \mathbb{R} | \quad \Delta^2(\lambda) = \frac{5}{12}\}$ *be labelled in the increasing order each other. Then, we have*

$$\lambda^-_{k,4n-2} \leq \eta_n \leq \lambda^+_{k,4n-2}, \quad \lambda^-_{k,4n} \leq \mu_n \leq \lambda^+_{k,4n}$$

for any $n \in \mathbb{N}$ *and* $k = 0, 1, 2, \ldots, N$. *Furthermore, we have*

$$\lambda^-_{k,4n-3} \leq \xi_{2n-1} \leq \lambda^+_{k,4n-3}, \quad \lambda^-_{k,4n-1} \leq \xi_{2n} \leq \lambda^+_{k,4n-1}$$

for any $n \in \mathbb{N}$ *and* $k = 0, 1, 2, \ldots, \ell_N$.

(viii) For $n \in \mathbb{N}$, *we put*

$$\lambda^-_n = \max_{0 \leq k \leq \ell_N} \lambda^-_{k,n} \quad \text{and} \quad \lambda^+_n = \min_{0 \leq k \leq \ell_N} \lambda^+_{k,n}.$$

Then, we have

$$\bigcup_{k=0}^{\ell_N} \sigma_{ac}(H_k) = \bigcup_{n=1}^{\infty} [\lambda_{n-1}^+, \lambda_n^-].$$

Especially, we have

$$\sigma_{ac}(H) = \begin{cases} \bigcup_{n=1}^{\infty} [\lambda_{n-1}^+, \lambda_n^-] & \text{if } N = 2\ell - 1, \\ \left(\bigcup_{n=1}^{\infty} [\lambda_{n-1}^+, \lambda_n^-]\right) \cup \sigma_{ac}(H_\ell) & \text{if } N = 2\ell. \end{cases}$$

(ix) For $n \in \mathbb{N}$, we put $\gamma_n := (\lambda_n^-, \lambda_n^+)$. Then, we have the followings:

(a) For $n \in \mathbb{N}$, we see that $\lambda_{0,4n}^- \neq \lambda_{0,4n}^+$ if and only if $\gamma_{4n} \neq \emptyset$.

(b) For $n \not\equiv 0 \pmod 4$, we see that $\gamma_n \neq \emptyset$ if and only if there does not exist $k \in \{1, 2, \ldots, \ell_N\}$ satisfying $\lambda_{k,n}^- = \lambda_{k,n}^+$.

3 Comparision

Let us compare our results with the results established in [Korotyaev and Lobanov, '07]. Kotoraev and Lobanov studied the spectral theory for periodic Schrödinger operators on zigzag carbon nanotube in the even case $N = 2m + 1$ for a fixed integer $m \geq 0$ such as

$$(\tilde{H} f_\omega)(x) = -f_\omega''(x) + q(x) f_\omega(x), \quad x \in (0,1),$$

$$\mathrm{Dom}(\tilde{H}) = \left\{ \bigoplus_{\omega \in \mathcal{Z}} f_\omega \in L^2(\Gamma^N) \;\middle|\; \begin{array}{l} \bigoplus_{\omega \in \mathcal{Z}} (-f_\omega'' + q f_\omega) \in L^2(\Gamma^N), \\ -f_{n,0,k}'(1) + f_{n,1,k}'(0) - f_{n,2,k-1}'(1) = 0, \\ f_{n,1,k}(0) = f_{n,0,k}(1) = f_{n,2,k-1}(1), \\ f_{n+1,0,k}'(0) - f_{n,1,k}'(1) + f_{n,2,k}'(0) = 0, \\ f_{n,1,k}(1) = f_{n+1,0,k}(0) = f_{n,2,k}(0) \\ \text{for} \quad n \in \mathbb{Z} \text{ and } k \in \mathbb{Z}_N \end{array} \right\}.$$

Recall that $s = e^{i\frac{2\pi}{N}}$. Korotyaev and Lobanov proved the unitarily equivalence $\tilde{H} \simeq \oplus_{k=1}^{N} \tilde{H}_k$, where $\tilde{H}_k$ is the following operator in $L^2(\tilde{\Gamma}^1)$ for $k = 1, 2, \ldots, N$:

$$(\tilde{H}_k f_\alpha)(x) = -f_\alpha''(x) + q(x) f_\alpha(x), \quad x \in (0,1), \quad \alpha \in \tilde{\mathcal{Z}}_1 := \mathbb{Z} \times \{0,1,2\},$$

$$\mathrm{Dom}(\tilde{H}_k) = \left\{ \bigoplus_{\alpha \in \tilde{\mathcal{Z}}_1} f_\alpha \in L^2(\Gamma^1) \;\middle|\; \begin{array}{l} \bigoplus_{\alpha \in \tilde{\mathcal{Z}}_1} (-f_\alpha'' + q f_\alpha) \in L^2(\Gamma^1), \\ -f_{n,0}'(1) + f_{n,1}'(0) - s^k f_{n,2}'(1) = 0, \\ f_{n,1}(0) = f_{n,0}(1) = s^k f_{n,2}(1), \\ f_{n+1,0}'(0) - f_{n,1}'(1) + f_{n,2}'(0) = 0, \\ f_{n,1}(1) = f_{n+1,0}(0) = f_{n,2}(0) \\ \qquad \text{for} \quad n \in \mathbb{Z} \end{array} \right\}.$$

The degenerate zigzag carbon nanotube $\tilde{\Gamma}^1$ can be seen in Fig. 7 (Compare with Fig. 6.).

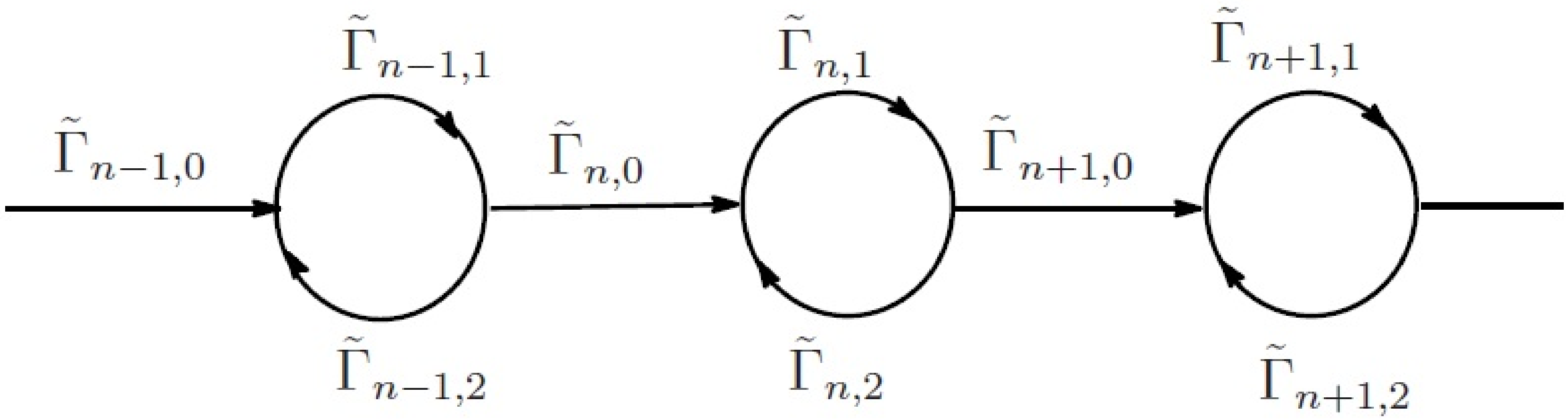


Fig. 7 The degenerate zigzag carbon nanotube $\tilde{\Gamma}^1$.

For $k = 0, 1, 2, \ldots, N-1$, define $F_0(\lambda) = 2\Delta^2(\lambda) + \frac{\theta_1'(\lambda)\varphi_1(\lambda)}{4} - 1$, $\xi_k = \frac{F_0 + s_k^2}{c_k}$, $\rho_k = s_k^2(1 - \xi_k^2)$ and $F_k^+ = c_k \xi_k + \sqrt{\rho_k}$.

Theorem 3.1 (Korotyaev and Lobanov, '07).
(i) For $k = 0, 1, 2, \ldots, N$, $\sigma(H_k) = \sigma_\infty(H_k) \cup \sigma_{ac}(H_k)$, where $\sigma_\infty(H_k) = \sigma_D(L)$ and $\sigma_{ac}(H_k) = \{\lambda |\ F_k^+(\lambda) \in [-1, 1]\}$.
(ii) For $k = 0, 1, 2, \ldots, N$, $\sigma_{ac}(H_k) = \sigma_{ac}(H_{N-k})$.
(iii) For $k = 0, 1, 2, \ldots, N$, there exists real sequence

$$\tilde{\lambda}_{k,0}^+ < \tilde{\lambda}_{k,1}^- \le \tilde{\lambda}_{k,1}^+ < \tilde{\lambda}_{k,2}^- \le \tilde{\lambda}_{k,2}^+ < \cdots < \tilde{\lambda}_{k,n}^- \le \tilde{\lambda}_{k,n}^+ < \cdots$$

such that

$$\sigma_{ac}(H_k) = \bigcup_{j=1}^{\infty} [\tilde{\lambda}_{k,j-1}^+, \tilde{\lambda}_{k,j}^-].$$

(iv) Theorem 3.3 in [Korotyaev and Lobanov, '07] reads that

$$\tilde{\lambda}^+_{0,0} < \tilde{\lambda}^-_{0,1} < \tilde{\lambda}^+_{0,1} < \tilde{\lambda}^-_{0,2} \le \tilde{\lambda}^+_{0,2} < \tilde{\lambda}^-_{0,3} < \tilde{\lambda}^+_{0,3} < \tilde{\lambda}^-_{0,4} \le \tilde{\lambda}^+_{0,4} < \cdots$$
$$< \tilde{\lambda}^-_{0,2n-1} < \tilde{\lambda}^+_{0,2n-1} < \tilde{\lambda}^-_{0,2n} \le \tilde{\lambda}^+_{0,2n} < \cdots .$$

(v) Theorem 1.4 in [Korotyaev and Lobanov, '07][*3] *reads that*

$$\tilde{\lambda}^+_{k,0} < \tilde{\lambda}^-_{k,1} \le \tilde{\lambda}^+_{k,1} < \tilde{\lambda}^-_{k,2} < \tilde{\lambda}^+_{k,2} < \tilde{\lambda}^-_{k,3} \le \tilde{\lambda}^+_{k,3} < \tilde{\lambda}^-_{k,4} < \tilde{\lambda}^+_{k,4} < \cdots \quad \text{if } k = \frac{N}{3},$$

$$\tilde{\lambda}^+_{k,0} < \tilde{\lambda}^-_{k,1} < \tilde{\lambda}^+_{k,1} < \tilde{\lambda}^-_{k,2} < \tilde{\lambda}^+_{k,2} < \tilde{\lambda}^-_{k,3} < \tilde{\lambda}^+_{k,3} < \tilde{\lambda}^-_{k,4} < \tilde{\lambda}^+_{k,4} < \cdots \quad \text{if } k \ne \frac{N}{3}$$

for $k = 1, 2, \ldots, N-1$.

---

*3 Note that $k = \frac{N}{3}$ is equivalent to $s_k = \sqrt{\frac{6}{8}}$.

Remark 3.2. *Theorem 1.8 implies that*

$$\lambda_{k,0}^{+} < \lambda_{k,1}^{-} \leq \lambda_{k,1}^{+} < \lambda_{k,2}^{-} < \lambda_{k,2}^{+} < \lambda_{k,3}^{-} \leq \lambda_{k,3}^{+} < \lambda_{k,4}^{-} < \lambda_{k,4}^{+} < \cdots$$

$$\text{if } k = \frac{N}{\pi} \sin^{-1} \sqrt{\frac{7}{8}},$$

$$\lambda_{k,0}^{+} < \lambda_{k,1}^{-} < \lambda_{k,1}^{+} < \lambda_{k,2}^{-} \leq \lambda_{k,2}^{+} < \lambda_{k,3}^{-} < \lambda_{k,3}^{+} < \lambda_{k,4}^{-} < \lambda_{k,4}^{+} < \cdots$$

$$\text{if } k = \frac{N}{6},$$

$$\lambda_{k,0}^{+} < \lambda_{k,1}^{-} < \lambda_{k,1}^{+} < \lambda_{k,2}^{-} < \lambda_{k,2}^{+} < \lambda_{k,3}^{-} < \lambda_{k,3}^{+} < \lambda_{k,4}^{-} < \lambda_{k,4}^{+} < \cdots$$

$$\text{if } k \neq \frac{N}{6}, \frac{N}{\pi} \sin^{-1} \sqrt{\frac{7}{8}}$$

for $k = 1, 2, \ldots, N-1$*. Compare this result with Theorem 1.8 (v).*

Open Problem

Does $k = 1, 2, \ldots, N-1$ satisfying $s_k = \sin \frac{\pi k}{N} = \sqrt{\frac{7}{8}}$ exist ?

This open problem was resolved as follows:

Lemma 3.3. *(Miyanishi, 8, September, 2015)*
We have $\sin^{-1}\sqrt{\frac{7}{8}} \notin \pi\mathbb{Q}$.

Remark 3.4. *Remark 3.2 combined with Lemma 3.3 implies the followings: For* $k = 1, 2, \ldots, \ell_N - 1$, *we have*

$$\lambda^+_{k,0} < \lambda^-_{k,1} < \lambda^+_{k,1} < \lambda^-_{k,2} \leq \lambda^+_{k,2} < \lambda^-_{k,3} < \lambda^+_{k,3} < \lambda^-_{k,4} < \lambda^+_{k,4} < \\ < \lambda^-_{k,5} < \lambda^+_{k,5} < \lambda^-_{k,6} \leq \lambda^+_{k,6} < \lambda^-_{k,7} < \lambda^+_{k,7} < \lambda^-_{k,8} < \lambda^+_{k,8} < \cdots \\ \text{if } k = \frac{N}{6},$$

$$\lambda^+_{k,0} < \lambda^-_{k,1} < \lambda^+_{k,1} < \lambda^-_{k,2} < \lambda^+_{k,2} < \lambda^-_{k,3} < \lambda^+_{k,3} < \lambda^-_{k,4} < \lambda^+_{k,4} < \cdots \\ \text{if } k \neq \frac{N}{6}.$$

4 Unperturbed Discriminant

In order to roughly understand Theorem 2.4, we consider the unperturbed case: $q \equiv 0$. Namely, we consider

$$D_0(0, \lambda) = \frac{9}{2} \cos^2 \sqrt{\lambda} - \frac{29}{8} + \frac{1}{8 \cos^2 \sqrt{\lambda}}, \tag{4}$$

$$D_0(k, \lambda) = \frac{36 \cos^4 \sqrt{\lambda} - 29 \cos^2 \sqrt{\lambda} + 1 + 4s_k^2}{4\sqrt{4 \cos^4 \sqrt{\lambda} - 4s_k^2 \cos^2 \sqrt{\lambda} + s_k^2}} \tag{5}$$

for $k = 1, 2, \ldots, \ell - 1$. In the case where $N = 2\ell$ and $\ell \in \mathbb{N}$, we additionally need to consider

$$\mathcal{D}_0(\ell, \lambda) = \frac{36 \cos^4 \sqrt{\lambda} - 29 \cos^2 \sqrt{\lambda} + 5}{4(2 \cos^2 \sqrt{\lambda} - 1)}. \tag{6}$$

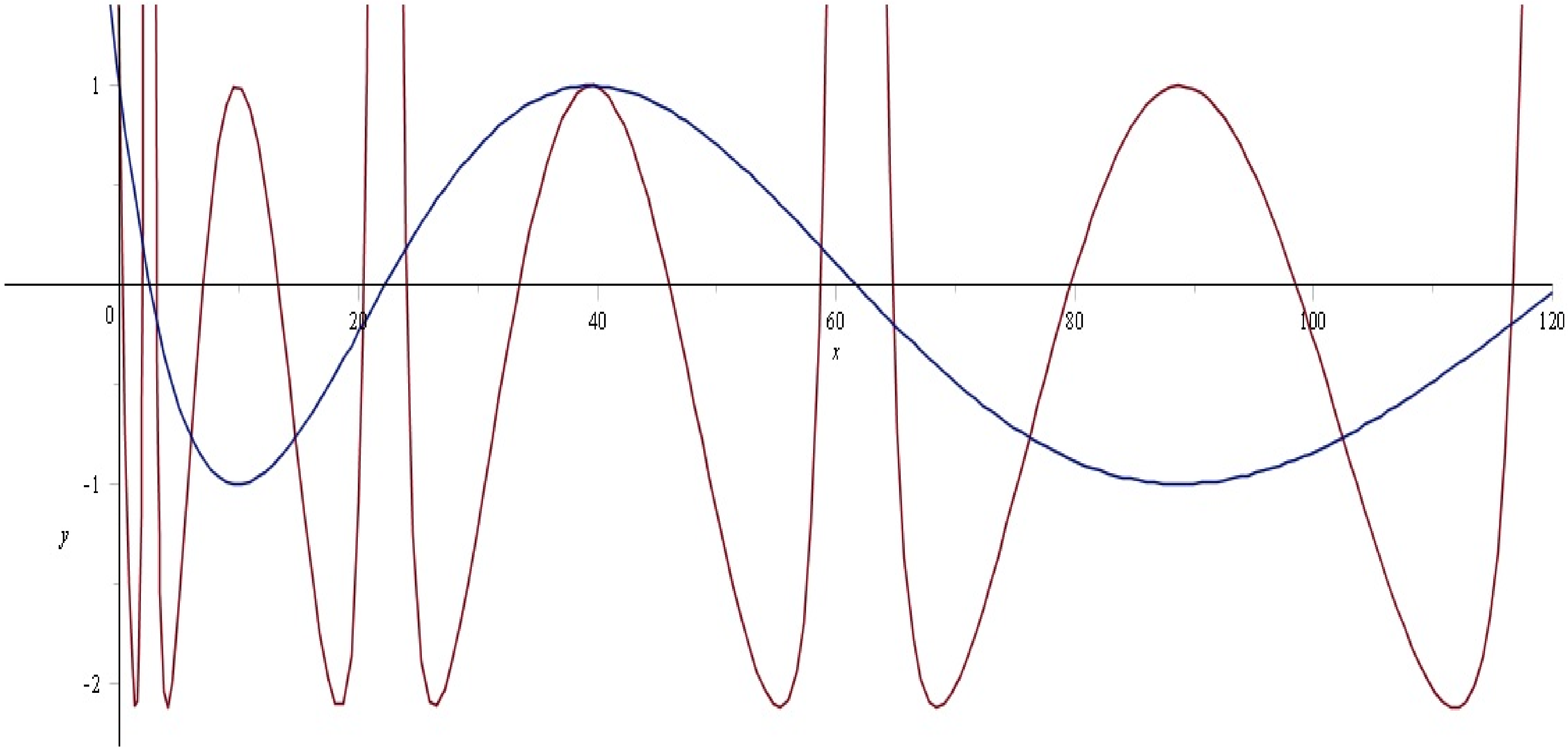


Fig. 8 The graph of $D_0(0, \lambda)$ and $\cos\sqrt{\lambda}$.

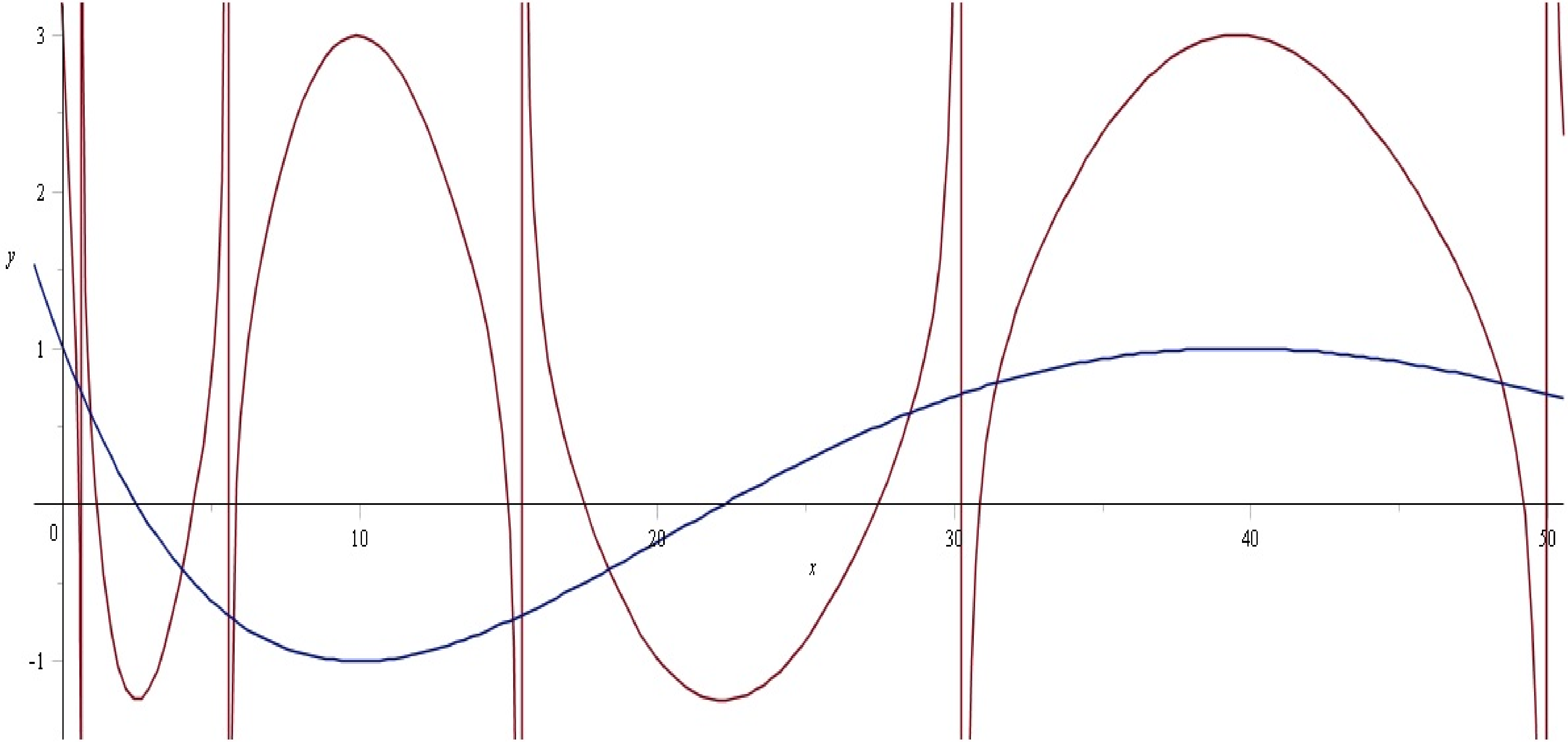


Fig. 9 The graph of $D_0(\ell, \lambda)$ and $\cos\sqrt{\lambda}$.

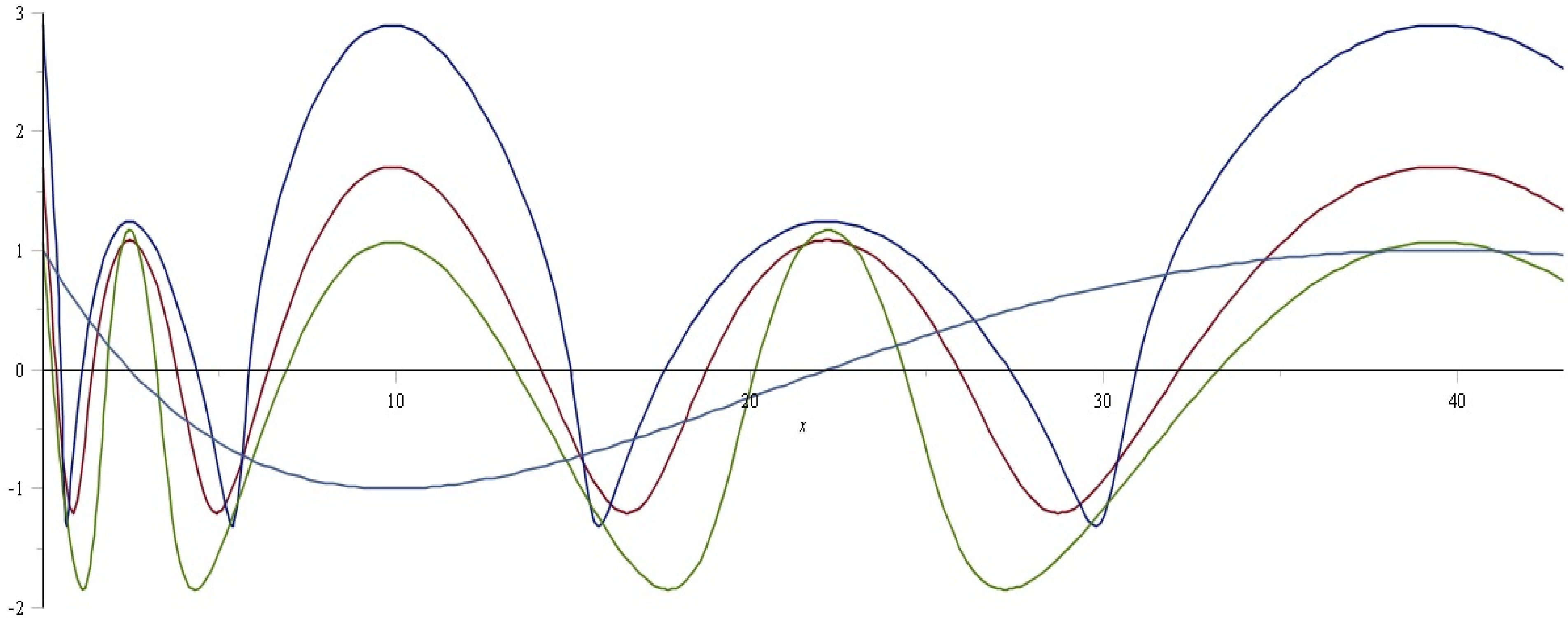


Fig. 10 The graph of $D_0(1, \lambda)$, $D_0(3, \lambda)$, $D_0(5, \lambda)$ in the case of $N = 11$ and $\cos\sqrt{\lambda}$.

5 Parts of the proof

We shall see that the perturbed discriminants $D(0,\lambda)$, $D(\ell,\lambda)$ and $\{D(k,\lambda)\}_{k=1}^{\ell-1}$ behaves in a similar way to the unperturbed discriminants $D_0(0,\lambda)$, $D_0(\ell,\lambda)$ and $\{D_0(k,\lambda)\}_{k=1}^{\ell-1}$ each other. We make sure this in only the case where $k=0$.

Lemma 5.1. *The discriminant $D(0,\lambda)$ has the following properties.*
(i) If $\lambda \in \sigma_D(L)$, then we have $D(0,\lambda) \geq 1$.
(ii) Let $\{\eta_n\}_{n=1}^{\infty} = \{\lambda \in \mathbb{R} | \quad \Delta(\lambda) = 0\}$ be labelled in the increasing order. Then, for each $n \in \mathbb{N}$, we have $D(0,\lambda) \to +\infty$ as $\lambda \to \eta_n \pm 0$.
(iii) If λ satisfies $\Delta^2(\lambda) = \frac{5}{12}$, then we have $D(0,\lambda) < -1$.
(iv) We have $D(0,\lambda) \to +\infty$ as $\lambda \to -\infty$.

We recall

$$D(k,\lambda) = \frac{2\Delta^2(\lambda)D(\lambda) + s_k^2}{\sqrt{4\Delta^4(\lambda) - 4\Delta^2(\lambda)s_k^2 + s_k^2}}.$$

The asymptotics of the fundamental solutions are well-known[*4]:

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

$$\begin{aligned}\varphi'(1,\lambda) = \cos\sqrt{\lambda} + \frac{1}{2\sqrt{\lambda}}\int_0^1 (\sin\sqrt{\lambda} + \sin\sqrt{\lambda}(1-2t))q(t)dt \\ +\mathcal{O}\left(\frac{e^{|\Im\sqrt{\lambda}|}}{|\lambda|}\right) \quad \text{as } |\lambda| \to \infty.\end{aligned}$$

---

*4 See [Poschel and Trubowitz, *Inverse Spectral Theory*].

Thus, Rouché's theorem is valid in the region appearing in the next two pages:

Theorem 5.2. *(Rouché's theorem[*5].) Suppose that $f(z)$ and $g(z)$ are meromorphic functions defined in the simply connected domain D, that C is simply closed contour in D, and that $f(z)$ and $g(z)$ have no zeroes or poles for $z \in C$. If the strict inequality $|f(z) + g(z)| < |f(z)| + |g(z)|$ holds for all $z \in C$, then we have $Z_f - P_f = Z_g - P_g$, where Z_f (Z_g, respectively) is the number of zeroes of $f(z)$ ($g(z)$, respectively) that lies inside C and P_f (P_g, respectively) is the number of zeroes of $f(z)$ ($g(z)$, respectively) that lies inside C.*

[*5] See [Mathews and Howell, *Complex Analysis for Mathematics and Engineering*]

Preparation for Rouché's theorem (1) We define

$$C_j^-(n) = \{\lambda \in \mathbb{C} | \quad \sqrt{\lambda} = n\pi + \gamma_j + ti, \quad -n \le t \le n\},$$

$$C_j^+(n) = \{\lambda \in \mathbb{C} | \quad \sqrt{\lambda} = n\pi + \gamma_{j+1} + ti, \quad -n \le t \le n\},$$

$$C_j^\times(n) = \{\lambda \in \mathbb{C} | \quad \sqrt{\lambda} = t + ni, \quad n\pi + \gamma_j \le t \le n\pi + \gamma_{j+1}\},$$

$$C_j^\div(n) = \{\lambda \in \mathbb{C} | \quad \sqrt{\lambda} = t - ni, \quad n\pi + \gamma_j \le t \le n\pi + \gamma_{j+1}\},$$

where $\gamma_0 = 0$, $\gamma_1 = \arccos\frac{1}{\sqrt{6}}$ and $\gamma_2 = \arccos\frac{1}{6}$ for $j = 0, 1$ and $n \in \mathbb{N}$. For $j = 2, 3$ and $n \in \mathbb{N}$, we define

$$C_j^-(n) = \{\lambda \in \mathbb{C} | \quad \sqrt{\lambda} = n\pi + \delta_j + ti, \quad -n \le t \le n\},$$

$$C_j^+(n) = \{\lambda \in \mathbb{C} | \quad \sqrt{\lambda} = n\pi + \delta_{j+1} + ti, \quad -n \le t \le n\},$$

$$C_j^\times(n) = \{\lambda \in \mathbb{C} | \quad \sqrt{\lambda} = t + ni, \quad n\pi + \delta_j \le t \le n\pi + \delta_{j+1}\},$$

$$C_j^\div(n) = \{\lambda \in \mathbb{C} | \quad \sqrt{\lambda} = t - ni, \quad n\pi + \delta_j \le t \le n\pi + \delta_{j+1}\},$$

where $\delta_2 = \arccos(-\frac{1}{6})$, $\delta_3 = \arccos(-\frac{1}{\sqrt{6}})$ and $\delta_4 = \pi$.

Furthermore, let $\Omega_j(n)$ be the region surrounded by

$$C_j(n) := C_j^{+}(n) - C_j^{\times}(n) - C_j^{-}(n) + C_j^{\div}(n)$$

for $j = 0, 1, 2, 3$ and $n \in \mathbb{N}$.
(2) For real sequences $\{a_n\}_{n=1}^{\infty}$ and $\{b_n\}_{n=1}^{\infty}$ satisfying $\sup_{n\in\mathbb{N}} a_n < \inf_{n\in\mathbb{N}} b_n$ and $a_n < b_n$ for every $n \in \mathbb{N}$, we define segments

$$C^{+}(b_n) = \{\lambda \in \mathbb{C} | \quad \sqrt{\lambda} = b_n + ti, \quad -n \le t \le n\},$$

$$C^{-}(a_n) = \{\lambda \in \mathbb{C} | \quad \sqrt{\lambda} = a_n - ti, \quad -n \le t \le n\},$$

$$C^{\times}(a_n, b_n) = \{\lambda \in \mathbb{C} | \quad \sqrt{\lambda} = ni + b_n + t(a_n - b_n), \quad 0 \le t \le 1\},$$

$$C^{\div}(a_n, b_n) = \{\lambda \in \mathbb{C} | \quad \sqrt{\lambda} = -ni + a_n + t(b_n - a_n), \quad 0 \le t \le 1\}$$

and $C(a_n, b_n) = C^{+}(b_n) + C^{\times}(a_n, b_n) + C^{-}(a_n) + C^{\div}(a_n, b_n)$ 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 $n \in \mathbb{N}$.

Lemma 5.3. *We have the followings:*
(I) For a fixed $c \in (-\frac{17}{8}, 1)$*, there exists some* $n_0 \in \mathbb{N}$ *satisfying the followings:*
(i) $D(0, \lambda) - c$ *has exactly one zero, counted with multiplicities, in* $\Omega_j(n)$ *for each* $j = 0, 1, 2, 3$ *and* $n_0 < n \in \mathbb{N}$.
(ii) $D(0, \lambda) - c$ *has* $(2 + 4n)$ *zeroes in* $\Omega(-(\gamma_2 + n\pi), \gamma_2 + n\pi)$ *for any* $n > n_0$*, where* $\gamma_2 = \arccos \frac{1}{6}$.
(iii) There are no other zeroes of $D(0, \lambda) - c$.

(II) For $c \in [1, \infty)$, there exists some $n_0 \in \mathbb{N}$ such that $D(\lambda) - c$ has 2 zeroes in $\Omega(n\pi + \frac{\pi}{3}, n\pi + \frac{2}{3}\pi)$ for each $n > n_0$.

(III) For $r \in (0, 1)$, there exists some $n_0 \in \mathbb{N}$ satisfying the followings:

- *(i) There are $(1 + 4n)$ zeroes of $D(0, \lambda) - 1$ in $\Omega(-(n\pi + r), n\pi + r)$ for each $n > n_0$.*
- *(ii) There are 2 zeroes of $D(0, \lambda) - 1$ in $\Omega(n\pi - r, n\pi + r)$ for each $n > n_0$.*
- *(iii) There are no other zeroes of $D(0, \lambda) - 1$ except for the zeroes stated in (II).*

(IV) For $r \in (-1,1)$, there exists some $n_0 \in \mathbb{N}$ satisfying the followings:

- *(i) There are 2 zeroes of $D(0,\lambda)+1$ in both regions $\Omega(\gamma_1 + n\pi - r, \gamma_1 + n\pi + r)$ and $\Omega(\delta_3 + n\pi - r, \delta_3 + n\pi + r)$ for $n > n_0$, where $\gamma_1 = \arccos \frac{1}{\sqrt{6}}$ and $\delta_3 = \arccos(-\frac{1}{\sqrt{6}})$.*
- *(ii) There are $4n$ zeroes of $D(0,\lambda)+1$ in $\Omega(-n\pi, n\pi)$ for $n > n_0$.*
- *(iii) There are no other zeroes of $D(0,\lambda)+1$.*

To be continued in ...

Schrödinger operatprs on a periodically broken zigzag carbon nanotube, submitted.

Thank you for your attention.

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