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Schrödinger operators on a zigzag supergraphene-based carbon nanotube

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QMath13

1 Introduction

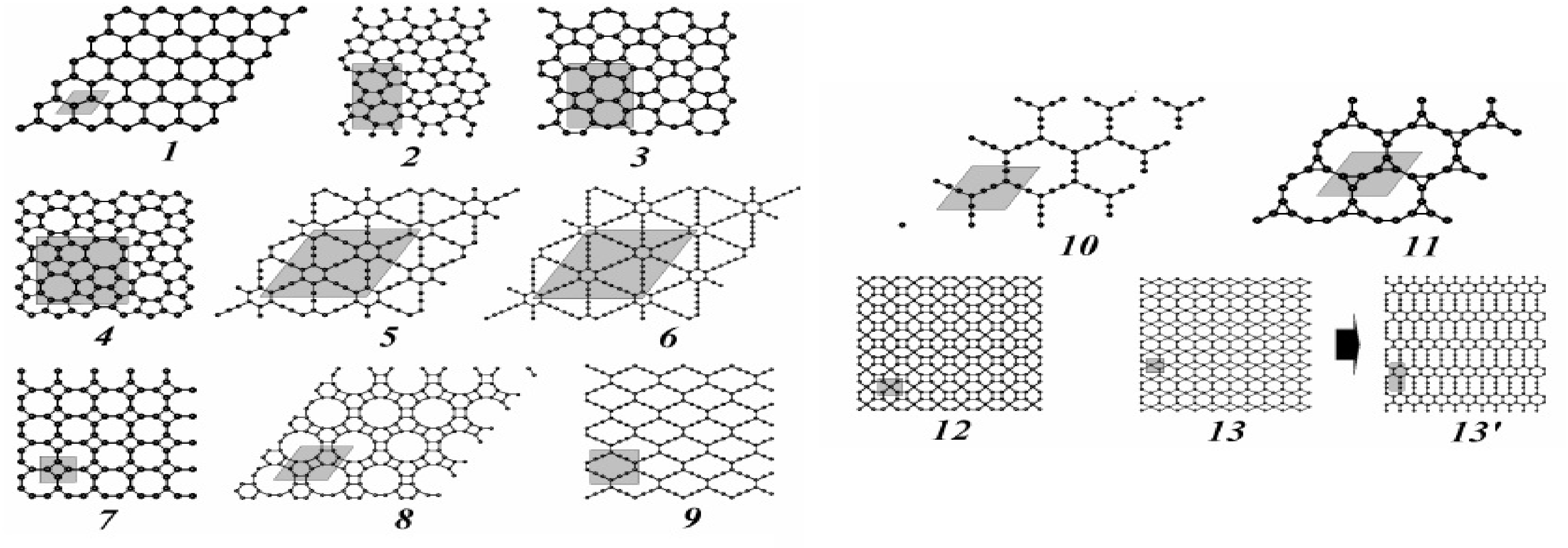

Fig. 1 Allotropes of Carbon [Enyashin and Ivanovskii, 2011].

(1) graphene (2),(3) pentaheptites (4) haecklites (5),(6) graphyne (10) supergraphene (12),(13) squarographene

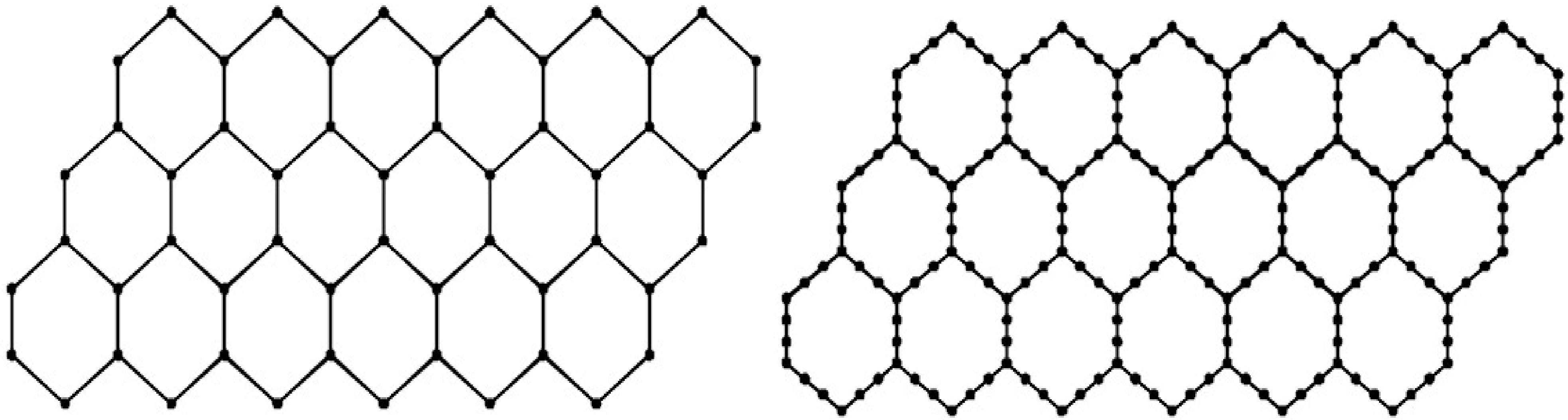

Fig. 2 graphene (left) and supergraphene (right)

Carbyne (Allotropes of Carbon) A Chain of Carbons

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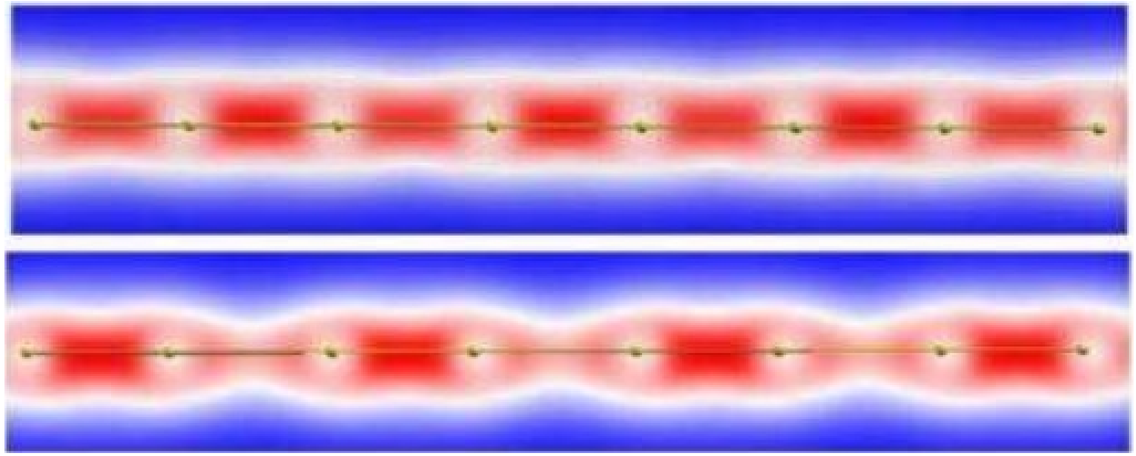


Fig. 3 ©Yakobson, et al. (2013)

Results of Yakobson's reseach group in Rice University:

- A carbyne has an extreme tensile stiffness: It is stiffer by a facor of two than graphene and carbon nanotubes.
- A carbyne is stronger than any other known material.

The aim of this talk is to examine the spectrum of periodic Schrödinger operators on a zigzag supergraphene-based carbon nanotube.

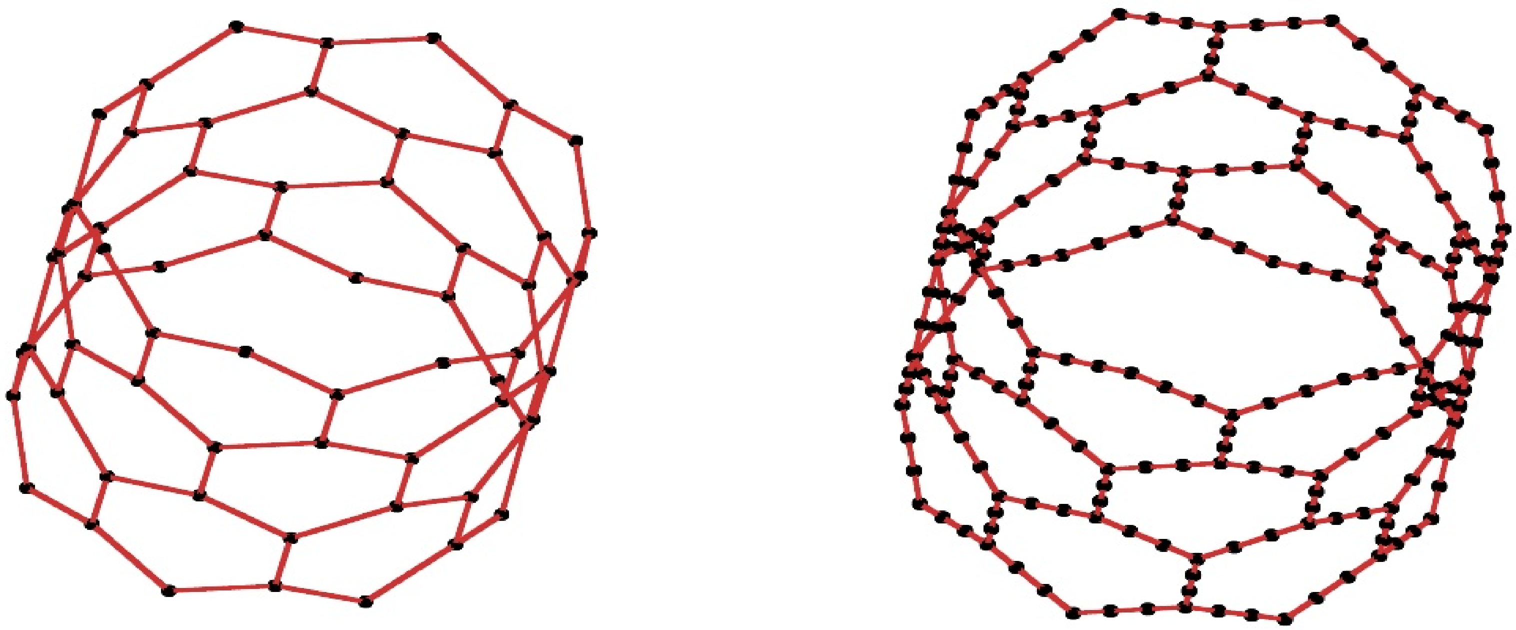
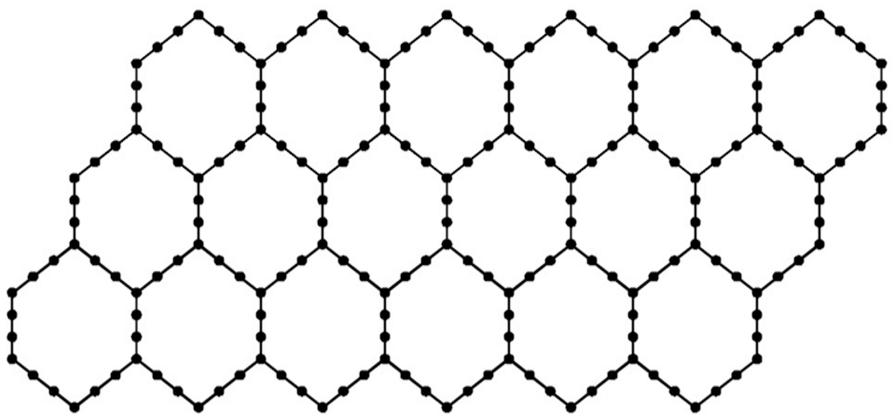


Fig. 4 a standard zigzag carbon nanotube(Left) and a zigzag supergraphene-based carbon nanotube Γ^N (Right).

Definition 1.1. *Let* $\mathbb{J} = \{1, 2, 3, ..., 9\}$*. For a fixed number* $N \in \mathbb{N}$*, we put* $\mathbb{Z}_N = \mathbb{Z}/(N\mathbb{Z}) = \{0, 1, 2, \ldots, N-1\}$*. For each* $\omega = (n, j, k) \in \mathcal{Z} := \mathbb{Z} \times \mathbb{J} \times \mathbb{Z}_N$*, we define* Γ_ω *as in the figure in the next slide.*



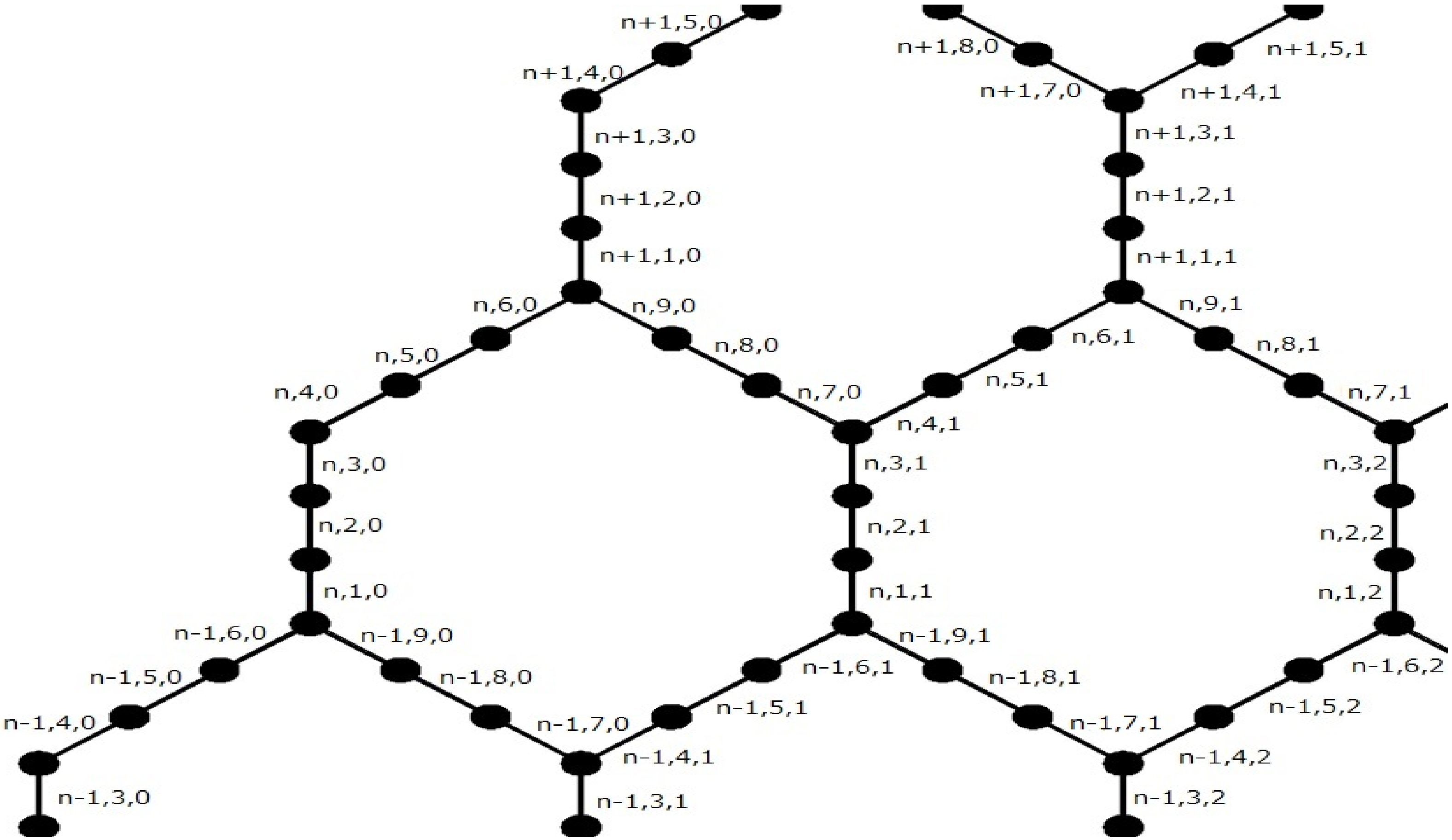


Fig. 5 The picture of $\Gamma_{n,j,k}$.

Taking the union $\Gamma^N := \cup_{\omega\in\mathcal{Z}}\Gamma_\omega$, we consider the Hilbert space $\mathcal{H}_N := L^2(\Gamma^N) = \oplus_{\omega\in\mathcal{Z}} L^2(\Gamma_\omega) = \oplus_{\omega\in\mathcal{Z}} L^2(0,1)$. For a real-valued function $q \in L^2(0,1)$, we consider a Schrödinger operator defined as

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

$$\begin{aligned}
&\mathrm{Dom}(H) \\
&= \left\{ \bigoplus_{\omega\in\mathcal{Z}} f_\omega \in \mathcal{H} \;\middle|\; \begin{array}{l}
\bigoplus_{\omega\in\mathcal{Z}}(-f''_\omega + qf_\omega) \in L^2(\Gamma^N), \\
f_{n,1,k}(1) = f_{n,2,k}(0), \quad f'_{n,1,k}(1) = f'_{n,2,k}(0), \\
f_{n,2,k}(1) = f_{n,3,k}(0), \quad f'_{n,2,k}(1) = f'_{n,3,k}(0), \\
f_{n,3,k}(1) = f_{n,4,k}(0) = f_{n,7,k-1}(0), \\
-f'_{n,3,k}(1) + f'_{n,4,k}(0) + f'_{n,7,k-1}(0) = 0, \\
f_{n,4,k}(1) = f_{n,5,k}(0), \quad f'_{n,4,k}(1) = f'_{n,5,k}(0), \\
f_{n,5,k}(1) = f_{n,6,k}(0), \quad f'_{n,5,k}(1) = f'_{n,6,k}(0), \\
f_{n,6,k}(1) = f_{n,9,k}(1) = f_{n+1,1,k}(0), \\
-f'_{n,6,k}(1) - f'_{n,9,k}(1) + f'_{n+1,1,k}(0) = 0, \\
f_{n,7,k}(1) = f_{n,8,k}(0), \quad f'_{n,7,k}(1) = f'_{n,8,k}(0), \\
f_{n,8,k}(1) = f_{n,9,k}(0), \quad f'_{n,8,k}(1) = f'_{n,9,k}(0) \\
\qquad\qquad \text{for} \quad n \in \mathbb{Z} \text{ and } k \in \mathbb{Z}_N
\end{array} \right\}.
\end{aligned}$$

Definition 1.2. *We call Γ^1 a degenerate zigzag supergraphene-based carbon nanotube.*

For convenience, we abbreviate $\Gamma_{n,j,1}$ as $\Gamma_{n,j}$ for each $(n, j) \in \mathcal{Z}_1 := \mathbb{Z} \times \mathbb{J}$.

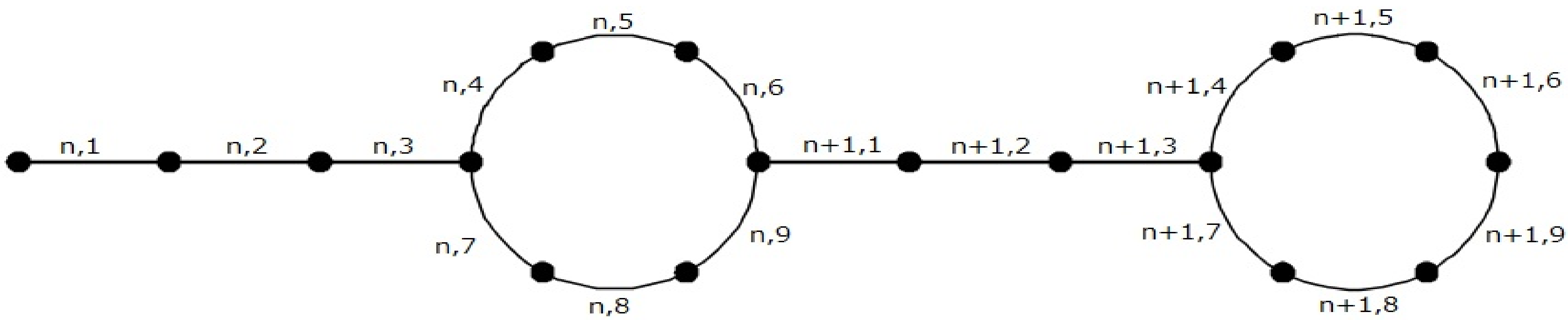


Fig. 6 A degenerate zigzag supergraphene-based CNT Γ^1.

For a fixed $N \in \mathbb{N}$, we put $s = e^{i\frac{2\pi}{N}}$. For $k = 1, 2, \ldots, N$, we consider the operator H_k in $\mathcal{H}_1 := L^2(\Gamma^1)$ defined as

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

$$\begin{aligned}
&\mathrm{Dom}(H_k) \\
&= \left\{ \bigoplus_{(n,j)\in\mathcal{Z}_1} u_{n,j} \in \mathcal{H}_1 \;\middle|\; \begin{array}{l}
\bigoplus_{(n,j)\in\mathcal{Z}_1}(-u''_{n,j} + qu_{n,j}) \in L^2(\Gamma^1), \\
u_{n,1}(1) = u_{n,2}(0), \quad u'_{n,1}(1) = u'_{n,2}(0), \\
u_{n,2}(1) = u_{n,3}(0), \quad u'_{n,2}(1) = u'_{n,3}(0), \\
u_{n,3}(1) = u_{n,4}(0) = s^k u_{n,7}(0), \\
-u'_{n,3}(1) + u'_{n,4}(0) + s^k u'_{n,7}(0) = 0, \\
u_{n,4}(1) = u_{n,5}(0), \quad u'_{n,4}(1) = u'_{n,5}(0), \\
u_{n,5}(1) = u_{n,6}(0), \quad u'_{n,5}(1) = u'_{n,6}(0), \\
u_{n,6}(1) = u_{n,9}(1) = u_{n+1,1}(0), \\
-u'_{n,6}(1) - u'_{n,9}(1) + u'_{n+1,1}(0) = 0, \\
u_{n,7}(1) = u_{n,8}(0), \quad u'_{n,7}(1) = u'_{n,8}(0), \\
u_{n,8}(1) = u_{n,9}(0), \quad u'_{n,8}(1) = u'_{n,9}(0) \\
\qquad\qquad \text{for} \quad n \in \mathbb{Z}
\end{array} \right\}.
\end{aligned}$$

- Utilizing the same method as [Korotyaev and Lobanov, '07], we obtain

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

  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 $\mathbb{R}$.

Review and Notation (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

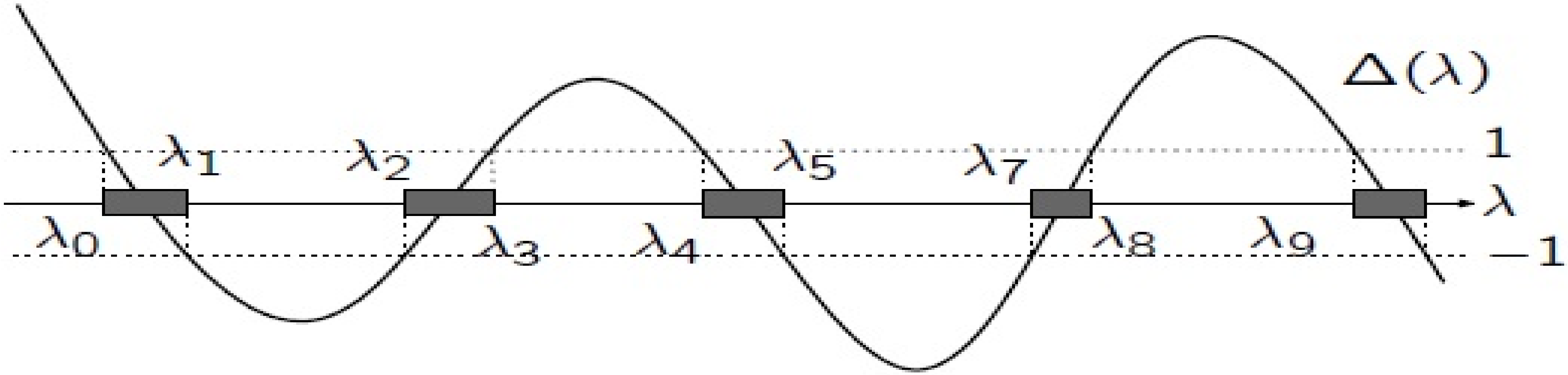
$$-y''(x,\lambda) + q(x)y(x,\lambda) = \lambda y(x,\lambda), \quad x \in \mathbb{R}, \tag{1}$$

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 $\sigma_D(L) := \{\mu_n\}_{n=1}^{\infty}$ be the Dirichlet spectrum, namely, the spectrum of the eigenvalue problem $-y'' + qy = \lambda y$ with $y(0) = y(1) = 0$. Recall $\mu_n \in [\lambda_{2n-1}, \lambda_{2n}]$ for each $n \in \mathbb{N}$.

(VI) $\sigma_{1/2}(L) := \{\lambda \in \mathbb{R} | \ \Delta = \frac{1}{2}\}$.
$\sigma_{-1/2}(L) := \{\lambda \in \mathbb{R} | \ \Delta = -\frac{1}{2}\}$.
$\sigma_{\pm 1/2}(L) := \sigma_{1/2}(L) \cup \sigma_{-1/2}(L)$.

2 $\sigma_\infty(H_k)$ and Discriminants of $\sigma_{ac}(H_k)$

We put $\Delta_- = \frac{\theta(1,\lambda)-\varphi'(1,\lambda)}{2}$.

- $\sigma_\infty(H)$; the set of eigenvalues of H with infinite multiplicities
- $\sigma_{ac}(H)$; the absolutely continuous spectrum of H.

If there exists some $\ell \in \mathbb{N}$ such that $(N,k) = (2\ell, \ell)$, then we define

$$D(\ell,\lambda) = D\left(\frac{N}{2}, \lambda\right)$$

$$= 144\Delta^6 - (216 + 16\Delta_-^2)\Delta^4 + (81 + 8\Delta_-^2)\Delta^2 - (1 + \Delta_-^2)$$

and $\sigma_{\ell,0} := \{\lambda \in \mathbb{R} |\ D(\ell,\lambda) = 0\}$.

If $(N,k) \neq (2\ell,\ell)$ for any $\ell \in \mathbb{N}$, then we define

$$D(k,\lambda) = \frac{1}{4\cos\frac{\pi k}{N}} \Big\{ 144\Delta^6 - (216 + 16\Delta_-^2)\Delta^4 + (81 + 8\Delta_-^2)\Delta^2 - (3 + s^k + s^{-k} + \Delta_-^2) \Big\}. \quad (2)$$

For $k = 1, 2, \ldots, N$, we notice that $\cos\frac{\pi k}{N} = 0$ is equivalent to $k = \frac{N}{2}$. Thus, (2) is well-defined.

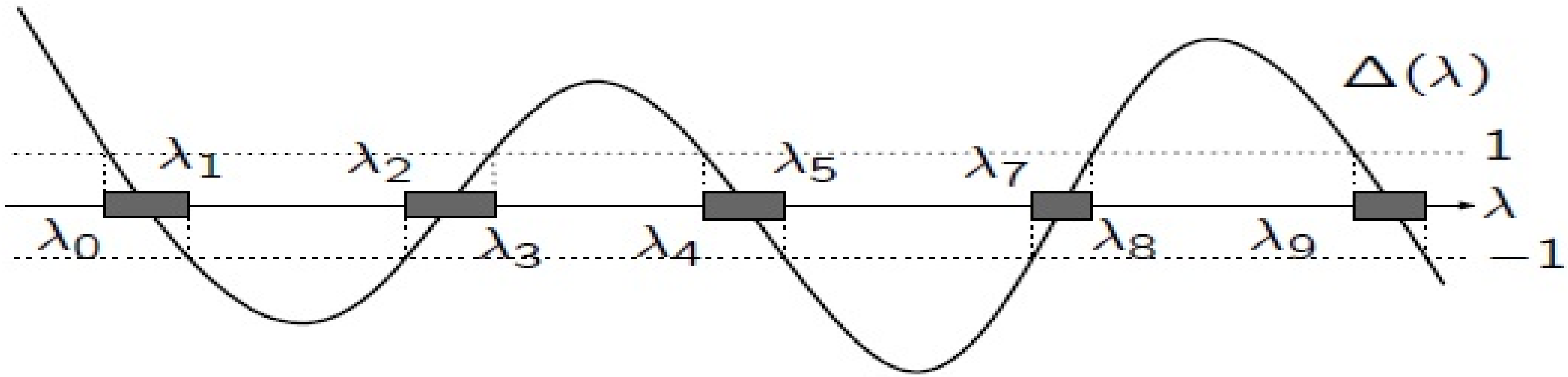
We have the followings:

Theorem 2.1. *For a fixed $\ell \in \mathbb{N}$, we obtain the followings:*
(i) If $N = 2\ell - 1$, then we have $\sigma(H_k) = \sigma_\infty(H_k) \cup \sigma_{ac}(H_k)$ for $k = 1, 2, \ldots, N$, where

$$\sigma_\infty(H_k) = \sigma_{\pm 1/2}(L) \cup \sigma_D(L)$$

and

$$\sigma_{ac}(H_k) = \{\lambda \in \mathbb{R} |\ |D(k, \lambda)| \le 1\}.$$



(ii) If $N = 2\ell$, then we have $\sigma(H_k) = \sigma_\infty(H_k) \cup \sigma_{ac}(H_k)$ for $k = 1, 2, \ldots, N$, where

$$\sigma_\infty(H_k) = \begin{cases} \sigma_{\pm 1/2}(L) \cup \sigma_D(L) & \text{if } k = \{1, \ldots, N\} \setminus \{N/2\}, \\ \sigma_{\pm 1/2}(L) \cup \sigma_D(L) \cup \sigma_{\ell,0} & \text{if } k = N/2, \end{cases}$$

and

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

Abbreviate $\theta(1, \lambda)$, $\theta'(1, \lambda)$, $\varphi(1, \lambda)$, $\varphi'(1, \lambda)$ to θ_1, θ'_1, φ_1, φ'_1.

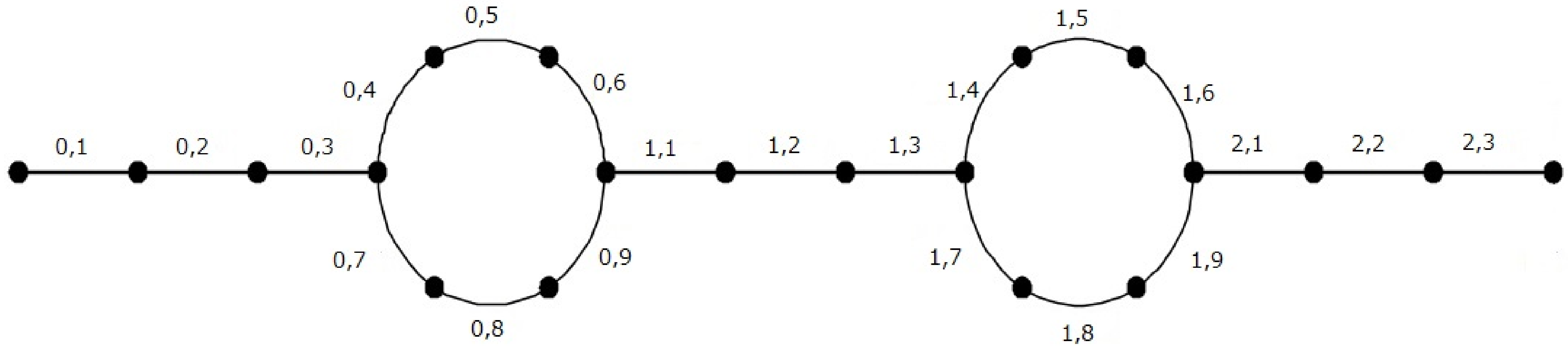
Lemma 2.2. *For a fixed $N \in \mathbb{N}$, we have*
$\sigma_{1/2}(L) \cup \sigma_{-1/2}(L) \subset \sigma_\infty(H_k)$ *for* $k = 1, 2, \ldots, N$.

Proof. (I) We 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

$$u_{0,4}^{(0)}(x,\lambda) = \varphi(x,\lambda), \quad u_{0,5}^{(0)}(x,\lambda) = v_1(x,\lambda),$$
$$u_{0,6}^{(0)}(x,\lambda) = v_2(x,\lambda), \quad u_{0,7}^{(0)}(x,\lambda) = -\varphi(x,\lambda),$$
$$u_{0,8}^{(0)}(x,\lambda) = -v_1(x,\lambda), \quad u_{0,9}^{(0)}(x,\lambda) = -v_2(x,\lambda)$$

and $u_{n,j}^{(0)}(x,\lambda) = 0$ for
$(n,j) \neq (0,4), (0,5), (0,6), (0,7), (0,8), (0,9)$.

Furthermore, we define $u^{(n)} = \{u^{(0)}_{m-n,j}\}_{(m,j)\in\mathcal{Z}_1}$. Then, we can directly check $\{u^{(n)}\}_{n\in\mathbb{Z}} \subset \mathrm{Dom}(H_0)$ and $H_0 u^{(n)} = \lambda u^{(n)}$ for any $n \in \mathbb{Z}$. Thus, we see that $\lambda \in \sigma_\infty(H_0)$. Hence, we have $\sigma_{1/2}(L) \subset \sigma_\infty(H_0)$.

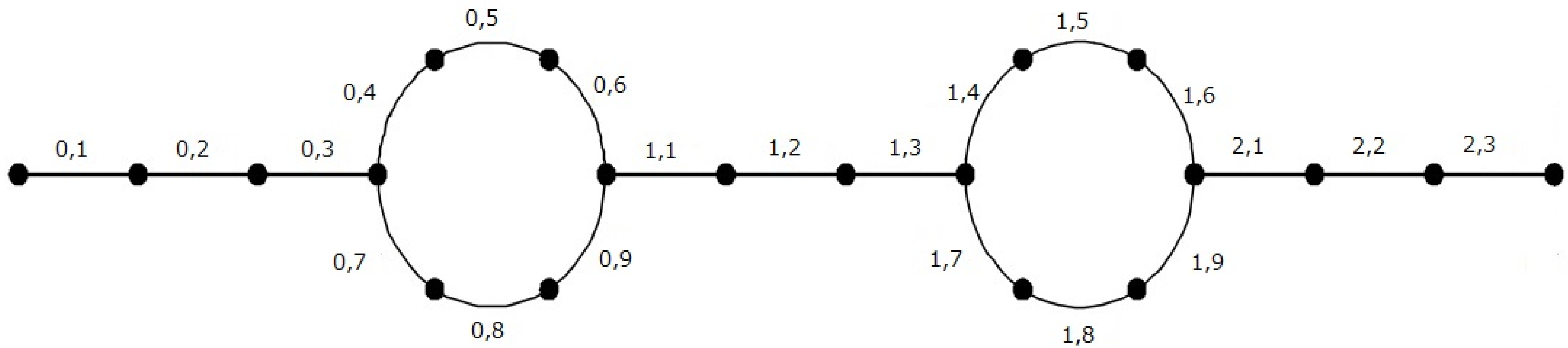


(b) Assume that $k = 1, 2, \ldots, N-1$. Then, we put
$\alpha_k = -1 + s^{-k}$, $\beta_k = \frac{1-s^{-k}}{1-s^k}$, $\gamma_k = -\frac{1-s^{-k}}{1-s^k}$,

$$u^{(0)}_{0,4}(x,\lambda) = \varphi(x,\lambda), \quad u^{(0)}_{0,5}(x,\lambda) = v_1(x,\lambda),$$
$$u^{(0)}_{0,6}(x,\lambda) = v_2(x,\lambda), \quad u^{(0)}_{0,7}(x,\lambda) = -s^{-k}\varphi(x,\lambda),$$
$$u^{(0)}_{0,8}(x,\lambda) = -s^{-k}v_1(x,\lambda), \quad u^{(0)}_{0,9}(x,\lambda) = -s^{-k}v_2(x,\lambda),$$
$$u_{1,1}(x,\lambda) = \alpha_k\varphi(x,\lambda), \quad u_{1,2}(x,\lambda) = \alpha_k v_1(x,\lambda),$$
$$u_{1,3}(x,\lambda) = \alpha_k v_2(x,\lambda), \quad u_{1,4}(x,\lambda) = \beta_k\varphi(x,\lambda),$$
$$u_{1,5}(x,\lambda) = \beta_k v_1(x,\lambda), \quad u_{1,6}(x,\lambda) = \beta_k v_2(x,\lambda),$$
$$u_{1,7}(x,\lambda) = \gamma_k\varphi(x,\lambda), \quad u_{1,8}(x,\lambda) = \gamma_k v_1(x,\lambda),$$
$$u_{1,9}(x,\lambda) = \gamma_k v_2(x,\lambda).$$

If $n \neq 1$ or $(n,j) \neq (0,4),(0,5),(0,6)$ is valid, then we define

$u_{n,j}^{(0)}(x,\lambda) = 0$. Then, for any $n \in \mathbb{Z}$, we see that $u^{(n)} := \{u_{m-n,j}^{(0)}\}_{(m,j)\in\mathcal{Z}_1}$ is an eigenvalue of H_k. So, we obtain $\sigma_{1/2}(L) \subset \sigma_\infty(H_k)$.



In a similar way, we can construct infinite many eigenfunctions for $\lambda \in \sigma_{-1/2}(L)$. $\square$

Lemma 2.3. *For a fixed $N \in \mathbb{N}$, we have $\sigma_D(L) \subset \sigma_\infty(H_k)$ for $k = 1, 2, \ldots, N$.*

A direct integral decomposition for H_k

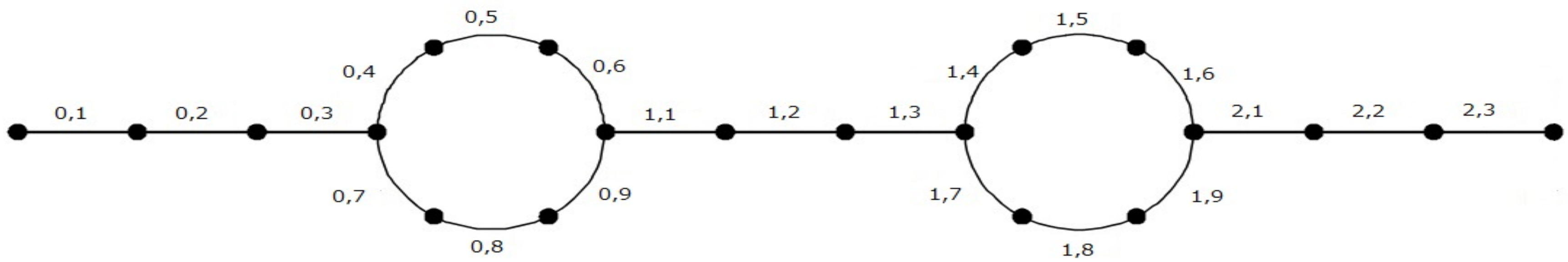
We examine $\sigma(H_k) \setminus (\sigma_{\pm 1/2}(L) \cup \sigma_D(L))$.
For $\mu \in [0, 2\pi)$, we define the Hilbert space $\mathcal{H}_\mu = \oplus_{j=1}^{9} L^2(\Gamma_{0,j})$. Prepare the Hilbert space

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

and the unitary operator $U : L^2(\Gamma^1) \to \mathcal{H}$ defined as

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

for $f = (f_n)_{n \in \mathbb{Z}} = (f_{n,j})_{(n,j) \in \mathcal{Z}_1} \in L^2(\Gamma)$. A fiber operator $H_k(\mu)$ in $\mathcal{H}_\mu$ for H_k is defined as follows:



$$(H_k(\mu)f_j)(x) = -f_j''(x) + q(x)f_j(x), \quad x \in (0,1) \simeq \Gamma^\circ_{0,j}, \quad j \in \mathbb{J},$$

$$\mathrm{Dom}(H_k(\mu)) = \left\{ \bigoplus_{j=1}^{9} f_j \in \mathcal{H}_\mu \;\middle|\; \begin{array}{l} \bigoplus_{j=1}^{9}(-f_j'' + qf_j) \in \mathcal{H}_\mu, \\ f_1(1) = f_2(0), \quad f_1'(1) = f_2'(0), \\ f_2(1) = f_3(0), \quad f_2'(1) = f_3'(0), \\ f_3(1) = f_4(0) = s^k f_7(0), \\ -f_3'(1) + f_4'(0) + s^k f_7'(0) = 0, \\ f_4(1) = f_5(0), \quad f_4'(1) = f_5'(0), \\ f_5(1) = f_6(0), \quad f_5'(1) = f_6'(0), \\ f_6(1) = f_9(1) = e^{i\mu} f_1(0), \\ -f_6'(1) - f_9'(1) + e^{i\mu} f_1'(0) = 0, \\ f_7(1) = f_8(0), \quad f_7'(1) = f_8'(0), \\ f_8(1) = f_9(0), \quad f_8'(1) = f_9'(0). \end{array} \right\}.$$

Then, we obtain a direct integral representation of H_k like

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

- $\{E_n(\mu)\}_{n\in\mathbb{N}}$; the sequence of the eigenvalues of $H_k(\mu)$
- $\mathcal{N}$; the set of natural numbers n such that $E_n(\mu)$ *does* depend on $\mu \in [0, 2\pi)$.
- $\sigma(H_k) = \sigma_\infty(H_k) \cup \sigma_{ac}(H_k)$, where

$$\sigma_\infty(H_k) = \bigcup_{n\in\mathcal{N}^c} \{E_n(\mu)\}$$

  and

$$\sigma_{ac}(H_k) = \bigcup_{n\in\mathcal{N}} \bigcup_{\mu\in[0,2\pi)} \{E_n(\mu)\}.$$

Proof of Theorem 2.1. We pick $\lambda \notin \sigma_{\pm 1/2}(L) \cup \sigma_D(L)$, arbitrarily. For this λ, we consider the characteristic equation $H_k(\mu)f = \lambda f$ for $0 \not\equiv f = (f_j)_{j=1}^9 \in \mathrm{Dom}(H_k(\mu))$. Namely, we consider the following system:

$$-f_j''(x) + q(x)f_j(x) = \lambda f_j(x), \quad x \in (0,1) \simeq \Gamma_{0,j}^\circ, \quad j \in \mathbb{J}, \tag{3}$$

$$f_1(1) = f_2(0), \quad f_2(1) = f_3(0), \quad f_4(1) = f_5(0), \tag{4}$$

$$f_5(1) = f_6(0), \quad f_7(1) = f_8(0), \quad f_8(1) = f_9(0), \tag{5}$$

$$f_3(1) = f_4(0) = s^k f_7(0), \quad f_6(1) = f_9(1) = e^{i\mu} f_1(0), \tag{6}$$

$$f_1'(1) = f_2'(0), \quad f_2'(1) = f_3'(0), \quad f_4'(1) = f_5'(0), \tag{7}$$

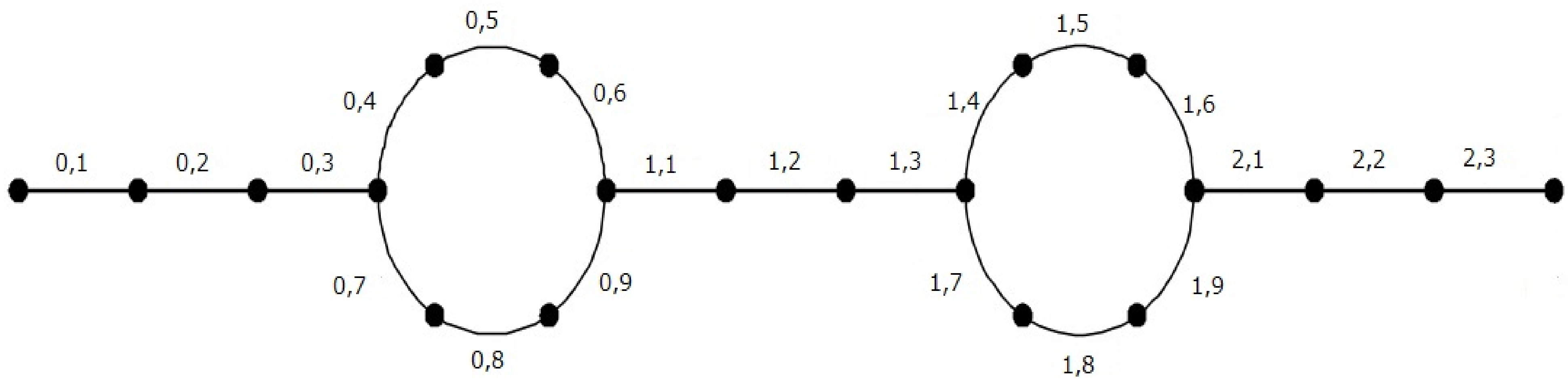
$$f_5'(1) = f_6'(0), \quad f_7'(1) = f_8'(0), \quad f_8'(1) = f_9'(0), \tag{8}$$

$$-f_3'(1) + f_4'(0) + s^k f_7'(0) = 0, -f_6'(1) - f_9'(1) + e^{i\mu} f_1'(0) = 0. \tag{9}$$

We first solve (3). It follows $\varphi_1 = \varphi(1,\lambda) \neq 0$ by $\lambda \notin \sigma_D(L)$. Thus, any solution to $-f'' + qf = \lambda f$ is given as

$$f(x,\lambda) = \theta(x,\lambda)f(0,\lambda) + \frac{\varphi(x,\lambda)}{\varphi_1}(f(1,\lambda) - \theta_1 f(0,\lambda)) \quad (10)$$

on $[0,1]$ for $\lambda \notin \sigma_D(L)$. Let us put $X_1 = f_1(0)$, $X_2 = f_2(0)$, $X_3 = f_3(0)$, $X_4 = f_4(0)$, $X_5 = f_5(0)$, $X_6 = f_6(0)$, $X_7 = f_8(0)$, $X_8 = f_9(0)$.



Putting $w(x,\lambda)=\theta(x,\lambda)-\frac{\theta(1,\lambda)}{\varphi(1,\lambda)}\varphi(x,\lambda)$, we have

$$f_1(x,\lambda)=w(x,\lambda)X_1+\frac{\varphi(x,\lambda)}{\varphi_1}X_2,\quad f_2(x,\lambda)=w(x,\lambda)X_2+\frac{\varphi(x,\lambda)}{\varphi_1}X_3,$$

$$f_3(x,\lambda)=w(x,\lambda)X_3+\frac{\varphi(x,\lambda)}{\varphi_1}X_4,\quad f_4(x,\lambda)=w(x,\lambda)X_4+\frac{\varphi(x,\lambda)}{\varphi_1}X_5,$$

$$f_5(x,\lambda)=w(x,\lambda)X_5+\frac{\varphi(x,\lambda)}{\varphi_1}X_6,\quad f_6(x,\lambda)=w(x,\lambda)X_6+\frac{\varphi(x,\lambda)}{\varphi_1}e^{i\mu}X_1,$$

$$f_7(x,\lambda)=w(x,\lambda)X_4+\frac{\varphi(x,\lambda)}{\varphi_1}X_7,\quad f_8(x,\lambda)=w(x,\lambda)X_7+\frac{\varphi(x,\lambda)}{\varphi_1}X_8,$$

$$f_9(x,\lambda)=w(x,\lambda)X_8+\frac{\varphi(x,\lambda)}{\varphi_1}e^{i\mu}X_1$$

due to (4), (5), (6) and (10).

Substituting these 9 formulas into (7), (8), (9), we obtain a system on $\{X_j\}_{j=1}^8$ as follows:

$$
\begin{aligned}
&X_1 - 2\Delta X_2 + X_3 = 0,\\
&X_2 - 2\Delta X_3 + X_4 = 0,\\
&X_3 - (2\theta_1 + \varphi_1')X_4 + X_5 + s^k X_7 = 0,\\
&X_4 - 2\Delta X_5 + X_6 = 0,\\
&e^{i\mu} X_1 + X_5 - 2\Delta X_6 = 0,\\
&s^{-k} X_4 - 2\Delta X_7 + X_8 = 0,\\
&e^{i\mu} X_1 + X_7 - 2\Delta X_8 = 0,\\
&-(2\varphi_1' + \theta_1)e^{i\mu} X_1 + e^{i\mu} X_2 + X_6 + X_8 = 0.
\end{aligned}
$$

Here, we recall Δ 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 $X_1, X_2, \ldots, X_8$:

$$\begin{pmatrix} 1 & -2\Delta & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & -2\Delta & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & -(2\theta_1+\varphi_1') & 1 & 0 & s^k & 0 \\ 0 & 0 & 0 & 1 & -2\Delta & 1 & 0 & 0 \\ e^{i\mu} & 0 & 0 & 0 & 1 & -2\Delta & 0 & 0 \\ 0 & 0 & 0 & s^{-k} & 0 & 0 & -2\Delta & 1 \\ e^{i\mu} & 0 & 0 & 0 & 0 & 0 & 1 & -2\Delta \\ -(2\varphi_1'+\theta_1)e^{i\mu} & e^{i\mu} & 0 & 0 & 0 & 1 & 0 & 1 \end{pmatrix}.$$

We have a dispersion relation

$$\begin{aligned} 0 &= e^{-i\mu}\det M_k(\lambda,\mu) \\ &= (4\Delta^2-1)\Big[4\cos\left(\frac{\pi k}{N}+\mu\right)\cos\frac{\pi k}{N} - 144\Delta^6 \\ &+(216+16\Delta_-^2)\Delta^4 - (8\Delta_-^2+81)\Delta^2 + 3 + s^k + s^{-k} + \Delta_-^2\Big]. \end{aligned}$$

Note that $4\Delta^2 - 1 \neq 0$ for $\lambda \notin \sigma_{\pm 1/2}(L)$. Thus, for $\lambda \notin \sigma_{\pm 1/2}(L) \cup \sigma_D(L)$, we see that $\det M_k(\lambda, \mu) = 0$ is equivalent to

$$4\cos\left(\frac{\pi k}{N} + \mu\right)\cos\frac{\pi k}{N}$$
$$= 144\Delta^6 - (216 + 16\Delta_-^2)\Delta^4 + (8\Delta_-^2 + 81)\Delta^2 - (3 + s^k + s^{-k} + \Delta_-^2).$$

This gives us a spectral discriminant $D(k, \lambda)$. □

We recall

$$D(k,\lambda) = \frac{1}{4\cos\frac{\pi k}{N}}\Big\{144\Delta^6 - (216 + 16\Delta_-^2)\Delta^4$$
$$+(81 + 8\Delta_-^2)\Delta^2 - (3 + s^k + s^{-k} + \Delta_-^2)\Big\}.$$

3 Absolutely continuous spectrum of H_k: Unperturbed case

In the unperturbed case, we obtain a spectral discriminant

$$D_0(k,\lambda) = \frac{1}{4\cos\frac{\pi k}{N}}\left\{144\cos^6\sqrt{\lambda} - 216\cos^4\sqrt{\lambda} + 81\cos^2\sqrt{\lambda} - \left(3 + 2\cos\frac{2\pi k}{N}\right)\right\}$$

for $k \in \{1, 2, \ldots, N\} \setminus \{N/2\}$.

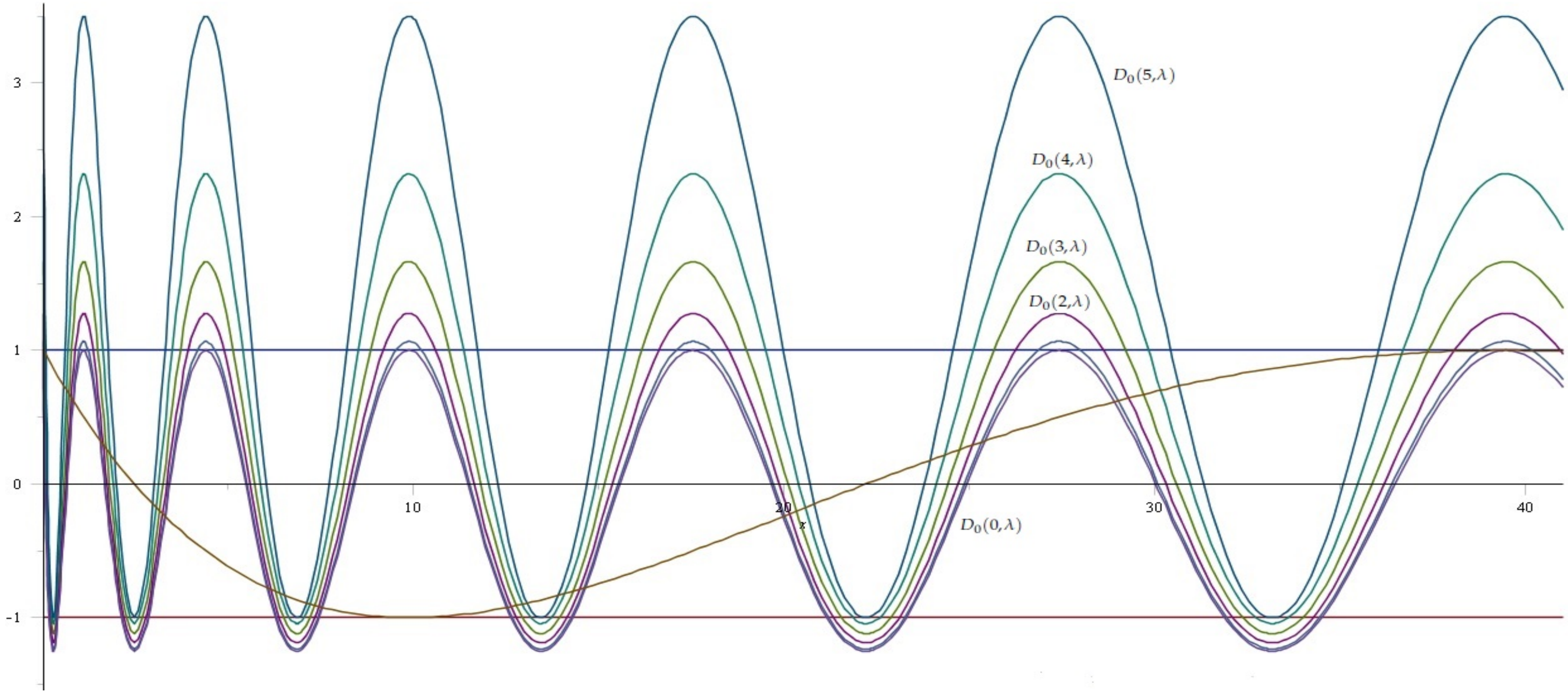


Fig. 7 The graph of $D_0(0,\lambda)$, $D_0(1,\lambda)$, $D_0(2,\lambda)$, $D_0(3,\lambda)$, $D_0(4,\lambda)$, $D_0(5,\lambda)$ and $\cos\sqrt{\lambda}$ in the case where $N = 15$. This picture hinted the results of the following Theorem 4.1. Namely, one can numerically expect that $\lambda^-_{k,2j} = \lambda^+_{k,2j}$ for $k = \frac{N}{3}$ and $\lambda^-_{k,2j-1} = \lambda^+_{k,2j-1}$ for $k = 0$ in the case where $q \equiv 0$.

4 Main Results

Theorem 4.1. *Let* $N = 2\ell - 1$ *or* $N = 2\ell$ *for a fixed* $\ell \in \mathbb{N}$.
(i) For $k = 0, 1, 2, \ldots, N$*, we have* $\sigma_{ac}(H_k) = \sigma_{ac}(H_{N-k})$.
Hence, we have

$$\sigma_{ac}(H) = \bigcup_{k=0}^{\ell-1} \sigma_{ac}(H_k).$$

(ii) For $k = 0, 1, 2, \ldots, \ell - 1$*, 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 $\sigma_{ac}(H_k) = \bigcup_{j=1}^{\infty} [\lambda_{k,j-1}^{+}, \lambda_{k,j}^{-}]$.

Namely, $\sigma_{ac}(H_k)$ has the band structure and hence we can define the jth band $\sigma_{k,j} = [\lambda^+_{k,j-1}, \lambda^-_{k,j}]$ and the jth spectral gap $\gamma_{k,j} = (\lambda^-_{k,j}, \lambda^+_{k,j})$ for each $j \in \mathbb{N}$.
(iii)

- *For $k \in \{1, 2, \dots, \ell - 1\}$, we have $\lambda^-_{k,2j} \neq \lambda^+_{k,2j}$ for every $j \in \mathbb{N}$.*
- *For $k \in \{0, 1, 2, \dots, \ell - 1\} \setminus \{\frac{N}{3}\}$, we have $\lambda^-_{k,2j-1} \neq \lambda^+_{k,2j-1}$.*
- *If $k \in \{0, 1, 2, \dots, \ell - 1\} \setminus \{0, \frac{N}{3}\}$, then every spectral gap of H_k is not degenerate, i.e., $\gamma_{k,j} \neq \emptyset$ is valid for all $j \in \mathbb{N}$.*

Asymptotic behavior of the spectral band edges

Notation For $q \in L^2(0,1)$, $j, n \in \mathbb{N}$ and $p = 1, 3, 5, 7, 9, 11$, we put

$$q_0 = \int_0^1 q(x)dx,$$

$$\hat{q}_n = \int_0^1 q(x)e^{2\pi i x}dx,$$

$$q_{c,j,n} = \int_0^1 (1-2t)^j q(t)\cos 2n\pi t dt,$$

$$q_{s,j,n} = \int_0^1 (1-2t)^j q(t)\sin 2n\pi t dt,$$

$$q_{s,j,n,p} = \int_0^1 (1-2t)^j q(t)\sin u^{\pm}_{\frac{N}{3},p+12n}(1-2t)dt.$$

Furthermore, for every $n \in \mathbb{N}$, we designate

$$u^{+}_{0,12n} = 2n\pi, \quad u^{\pm}_{0,12n+2} = \frac{\pi}{3} + 2n\pi, \quad u^{\pm}_{0,12n+4} = \frac{2}{3}\pi + 2n\pi,$$

$$u^{\pm}_{0,12n+6} = \pi + 2n\pi, \quad u^{\pm}_{0,12n+8} = \frac{4}{3}\pi + 2n\pi,$$

$$u^{\pm}_{0,12n+10} = \frac{5}{3}\pi + 2n\pi, \quad u^{-}_{0,12n+12} = 2\pi + 2n\pi,$$

$$u^{\pm}_{\frac{N}{3},12n+1} = 2n\pi + \frac{\pi}{6}, \quad u^{\pm}_{\frac{N}{3},12n+3} = \frac{\pi}{2} + 2n\pi,$$

$$u^{\pm}_{\frac{N}{3},12n+5} = \frac{5}{6}\pi + 2n\pi, \quad u^{\pm}_{\frac{N}{3},12n+7} = \frac{7}{6}\pi + 2n\pi,$$

$$u^{\pm}_{\frac{N}{3},12n+9} = \frac{3}{2}\pi + 2n\pi, \quad u^{\pm}_{\frac{N}{3},12n+11} = \frac{11}{6}\pi + 2n\pi.$$

Then, we have the following results for $k = 0, 1, 2, \ldots, \ell - 1$.

Theorem 4.2. *(i) Edges of even-numbdered spectral gaps behave as follows:*
(a) Let $k = 1, 2, \ldots, \ell - 1$. For $p = 1, 2, 3, 4, 5, 6$, we have

$$\lambda^{\pm}_{k,12n+2p} = (u^{\pm}_{k,12n+2p})^2 + q_0 + o\left(\frac{1}{n}\right) \quad \text{as } n \to \infty.$$

(b) Let $k = 0$. Then, we have

$$\lambda^{\pm}_{0,12n+p} = (u^{\pm}_{0,12n+p})^2 + q_0 + o\left(\frac{1}{n}\right) \quad \text{for } p = 2, 4, 8, 10,$$

$$\lambda^{\pm}_{0,12n+12} = 4(n+1)^2\pi^2 + q_0 \pm \sqrt{|\hat{q}_{2n+2}|^2 - \frac{8}{27} q^2_{s,0,2n+2} + o\left(\frac{1}{n}\right)} + \mathcal{O}\left(\frac{1}{n}\right),$$

$$\lambda^{\pm}_{0,12n+6} = (2n+1)^2\pi^2 + q_0 \pm \sqrt{|\hat{q}_{2n+1}|^2 - \frac{8}{27} q^2_{s,0,2n+1} + o\left(\frac{1}{n}\right)} + \mathcal{O}\left(\frac{1}{n}\right)$$

as $n \to \infty$.

(ii) Edges of odd-numbdered spectral gaps behave as follows:

(a) Let $k \neq \frac{N}{3}$ *or* q *be even. Then, for* $p = 1, 3, 5, 7, 9, 11$, *we have*

$$\lambda^{\pm}_{k,12n+p} = (u^{\pm}_{k,12n+p})^2 + q_0 + o\left(\frac{1}{n}\right) \quad \text{as } n \to \infty.$$

(b) Let $k = \frac{N}{3}$ *and* q *be not even. For* $p = 3, 9$, *we have*

$$\lambda^{\pm}_{\frac{N}{3},p+12n} = (u^{\pm}_{\frac{N}{3},p+12n})^2 + q_0 \pm \frac{\sqrt{789}}{108}\sqrt{q^2_{s,0,n,p} + o\left(\frac{1}{n}\right)} + o\left(\frac{1}{n}\right)$$

as $n \to \infty$. *For* $p = 1, 5, 7, 11$, *we have*

$$\lambda^{\pm}_{\frac{N}{3},p+12n} = (u^{+}_{\frac{N}{3},1+12n})^2 + q_0 \pm \frac{411}{1944}\sqrt{q^2_{s,0,n,p} + o\left(\frac{1}{n}\right)} + o\left(\frac{1}{n}\right)$$

as $n \to \infty$.

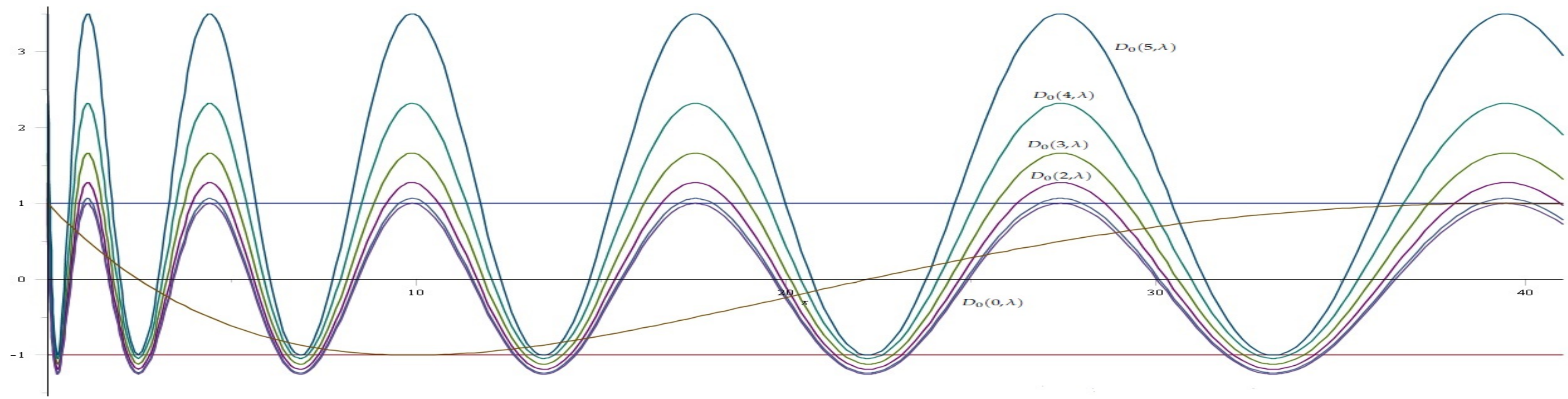
Absence of spectral gaps

Theorem 4.3. *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 $\frac{N}{3} \in \mathbb{N}$ *and* q *is even, then we have*

$\gamma_{\frac{N}{3},12n-11} = \gamma_{\frac{N}{3},12n-7} = \gamma_{\frac{N}{3},12n-5} = \gamma_{\frac{N}{3},12n-1} = \emptyset$.



5 Proof of Theorems

Discriminant of $z^3 + pz + q = 0$: $\mathcal{D} = -(4p^3 + 27q^2)$

- If $\mathcal{D} > 0$, then $z^3 + pz + q = 0$ has three distinct real roots.
- If $\mathcal{D} = 0$, then at least 2 roots of $z^3 + pz + q = 0$ coincide, and any root is real.
- If $\mathcal{D} < 0$, then $z^3 + pz + q = 0$ has 1 real root and 2 complex conjugate roots.

François Viète's solution to a cubic equation (16th century)

If $\mathcal{D} > 0$, then the solutions to $z^3 + pz + q = 0$ ($p < 0$, $q \in \mathbb{R}$) is given by

$$\alpha_k = 2\sqrt{-\frac{p}{3}} \cos\left\{\frac{1}{3}\arccos\left(\frac{3q}{2p}\sqrt{\frac{-3}{p}}\right) - \frac{2\pi}{3}k\right\}, k = 0, 1, 2.$$

We examine the asymptotics for zeroes of $D(k,\lambda)=-1$, which is equivalent to

$$\Delta^6-\left(\frac{3}{2}+\frac{\Delta_-^2}{9}\right)\Delta^4+\left(\frac{9}{16}+\frac{\Delta_-^2}{18}\right)\Delta^2$$
$$-\frac{1}{144}\left(3+2\cos\frac{2\pi k}{N}-4\cos\frac{\pi k}{N}+\Delta_-^2\right)=0.$$

Putting $\Delta^2=z+\left(\frac{1}{2}+\frac{\Delta_-^2}{27}\right)$, this is moreover equivalent to

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

Here, we put $f_k(-1)=8c_k^2-8c_k-7$ and $c_k=\cos\frac{\pi k}{N}$ for $k=0,1,\ldots,\ell-1$.

We consider its discriminant $D_k^- = D_k^-(\lambda) = 4p_-^3 - 27q_-^2$, where

$$p_- = \frac{3}{16} + \frac{\Delta_-^2}{18} + \frac{\Delta_-^4}{243}, \; q_- = \frac{f_k(-1)}{288} + \frac{\Delta_-^2}{9} \underbrace{\left(\frac{1}{8} + \frac{\Delta_-^2}{54} + \frac{2\Delta_-^4}{2187}\right)}_{\clubsuit}.$$

Let $q_{\frac{N}{3},-}$ be the q_- for $k = \frac{N}{3}$. It follows by straightforward calculations that $D_{\frac{N}{3}}^- = \frac{3}{64}\Delta_-^2 + \frac{1}{144}\Delta_-^4 + \frac{1}{2916}\Delta_-^6$ and

$$D_k^- = D_{\frac{N}{3}}^- - \frac{1}{48}\left(c_k - \frac{1}{2}\right)^2 \left\{\left(c_k - \frac{1}{2}\right)^2 - \frac{9}{4} + 8\Delta_-^2 \times (\clubsuit)\right\}.$$

Lemma 5.1. *(i) If* $k = \frac{N}{3}$ *and* q *is even, then we have* $D^{-}_{\frac{N}{3}} = 0$*.*
(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* $\lambda \geq \lambda_0$*.*

In the case of $D^{-}_{k} > 0$, we can construct Viéte's solution to $D(k, \lambda) = -1$:

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

as $\lambda \to +\infty$.

To be continued in ...

Schrödinger operators on a zigzag supergraphene-based carbon nanotube, submitted.

Thank you for your attention.

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