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Schrödinger operators on a zigzag  
supergraphene-based carbon nanotube

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QMath13

# 1 Introduction

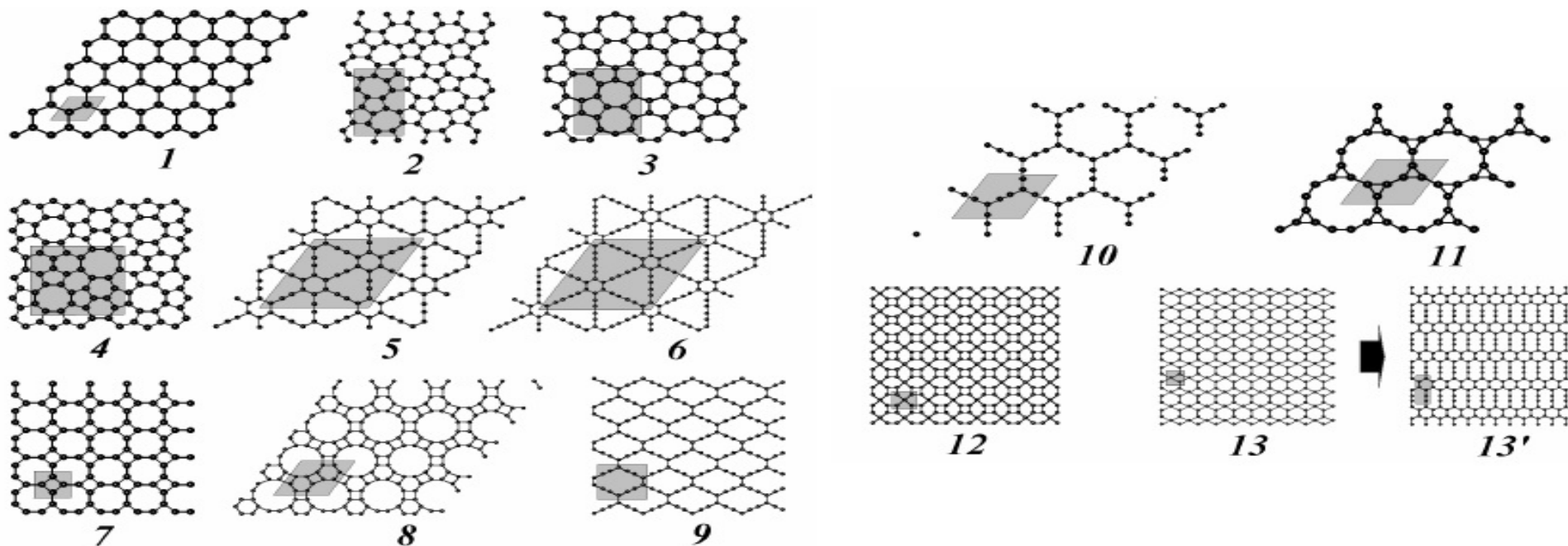


Fig. 1 Allotropes of Carbon [Enyashin and Ivanovskii, 2011].

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

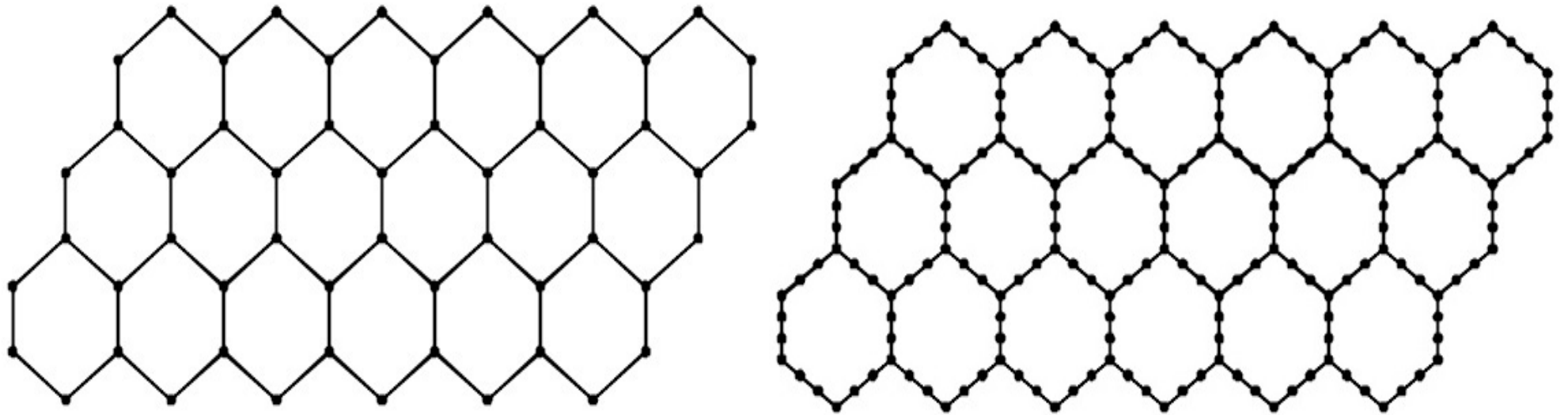


Fig. 2 graphene (left) and supergraphene (right)

Carbyne (Allotropes of Carbon) A Chain of Carbons

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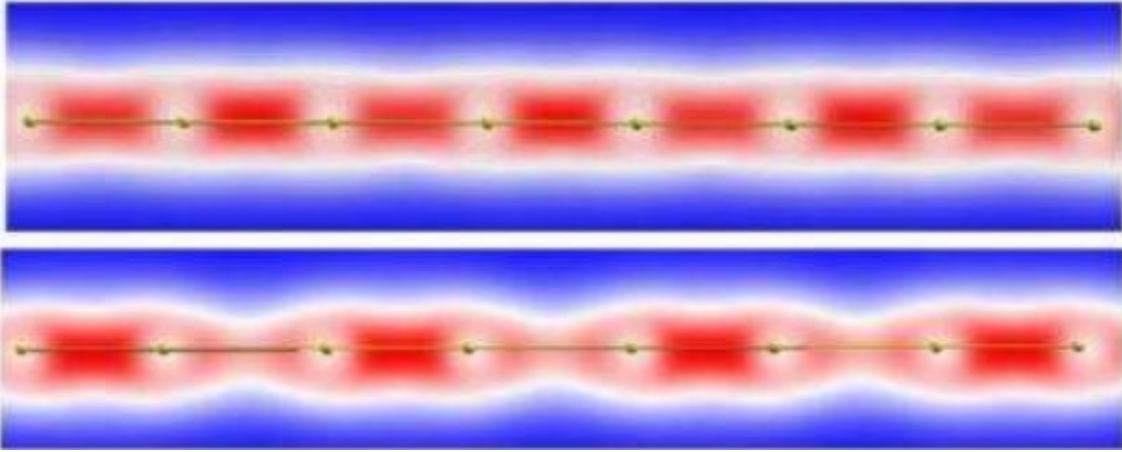


Fig. 3 ©Yakobson, et al. (2013)

Results of Yakobson's research group in Rice University:

- A carbyne has an extreme tensile stiffness: It is stiffer by a factor 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.

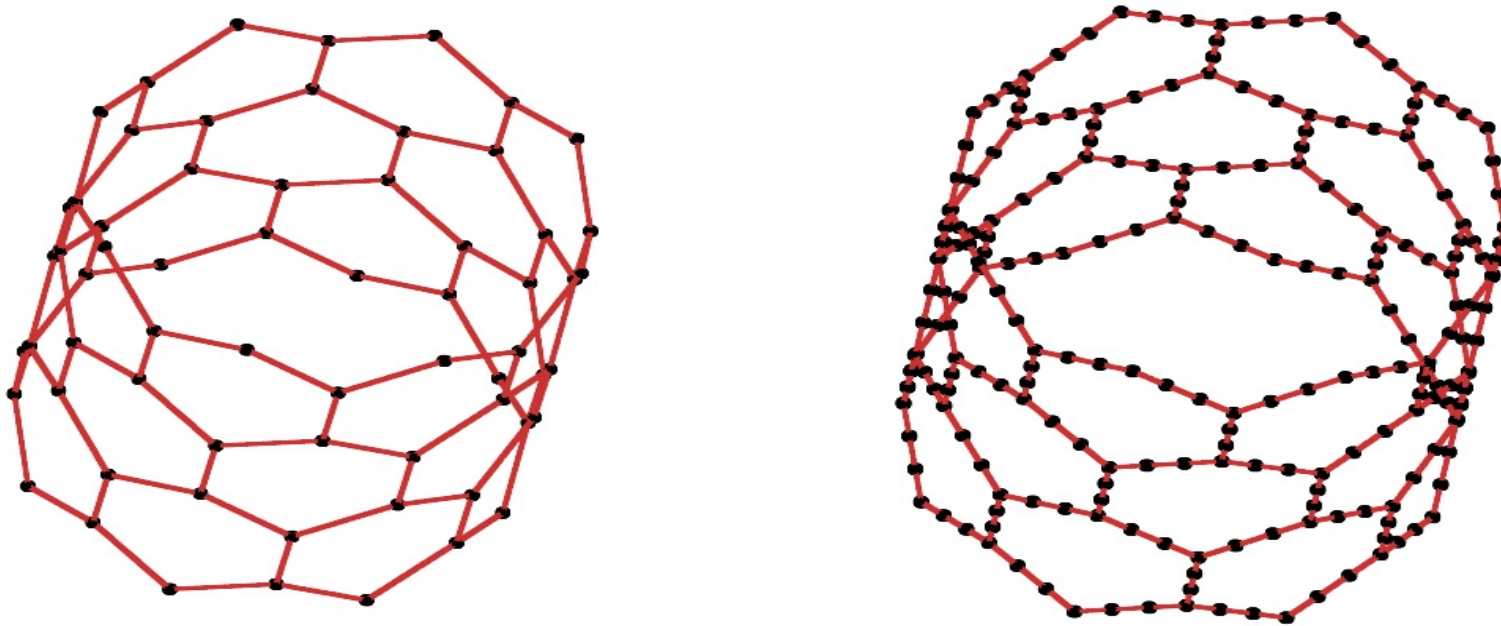
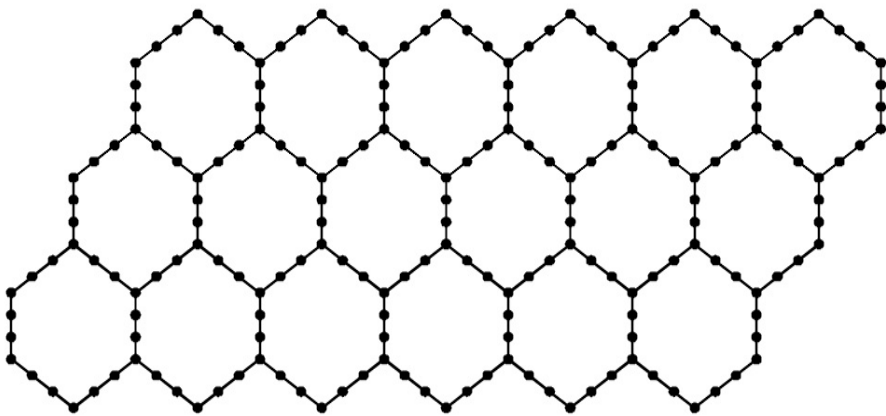


Fig. 4 a standard zigzag carbon nanotube(Left) and a zigzag supergraphene-based carbon nanotube  $\Gamma^N$  (Right).

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



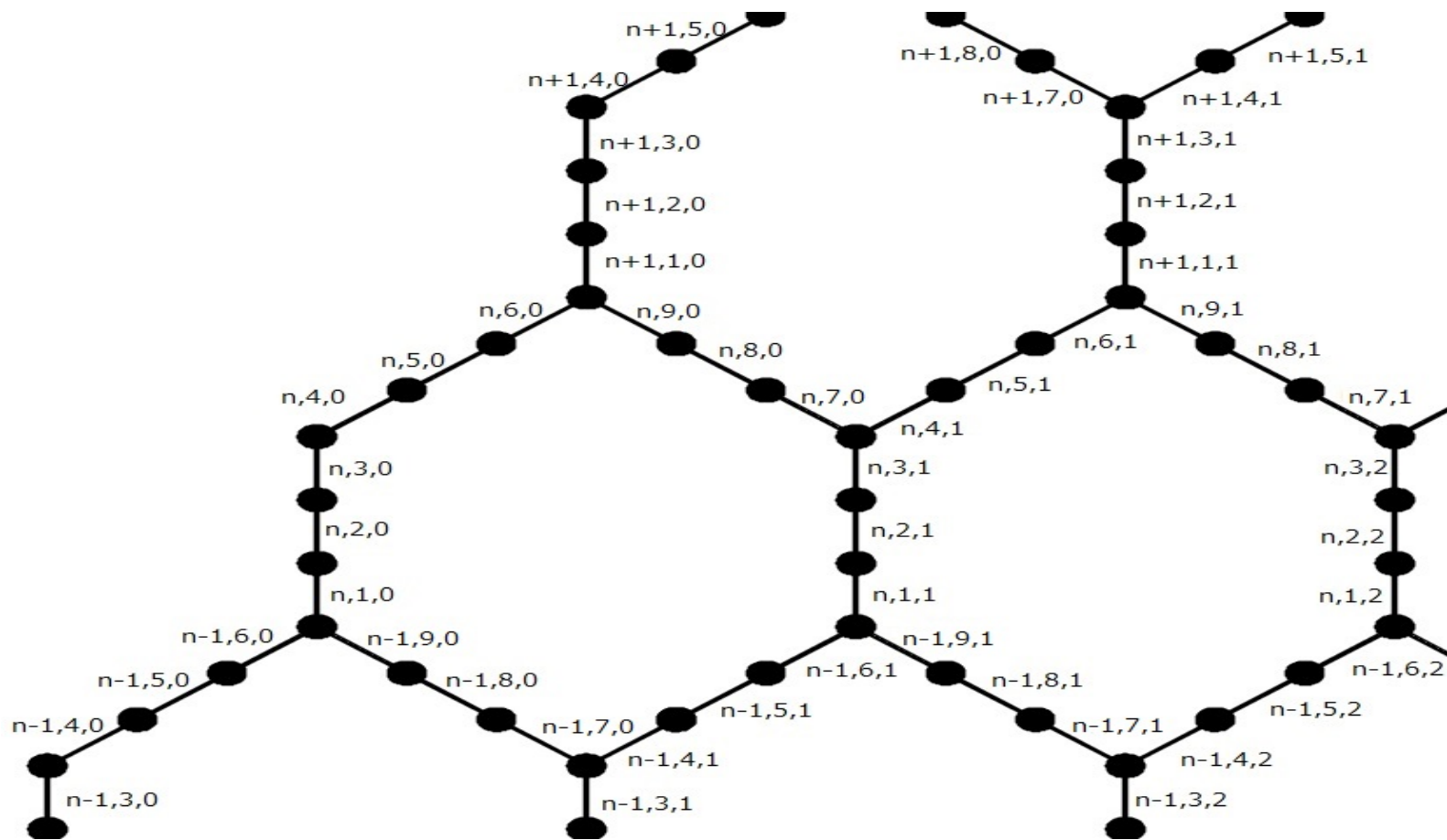


Fig. 5 The picture of  $\Gamma_{n,j,k}$ .

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

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

Dom( $H$ )

$$= \left\{ \bigoplus_{\omega \in \mathcal{Z}} f_\omega \in \mathcal{H} \mid \begin{array}{l} \bigoplus_{\omega \in \mathcal{Z}} (-f''_\omega + qf_\omega) \in L^2(\Gamma^N), \\ f_{n,1,k}(1) = f_{n,2,k}(0), \quad f'_{n,1,k}(1) = f'_{n,2,k}(0), \\ f_{n,2,k}(1) = f_{n,3,k}(0), \quad f'_{n,2,k}(1) = f'_{n,3,k}(0), \\ f_{n,3,k}(1) = f_{n,4,k}(0) = f_{n,7,k-1}(0), \\ -f'_{n,3,k}(1) + f'_{n,4,k}(0) + f'_{n,7,k-1}(0) = 0, \\ f_{n,4,k}(1) = f_{n,5,k}(0), \quad f'_{n,4,k}(1) = f'_{n,5,k}(0), \\ f_{n,5,k}(1) = f_{n,6,k}(0), \quad f'_{n,5,k}(1) = f'_{n,6,k}(0), \\ f_{n,6,k}(1) = f_{n,9,k}(1) = f_{n+1,1,k}(0), \\ -f'_{n,6,k}(1) - f'_{n,9,k}(1) + f'_{n+1,1,k}(0) = 0, \\ f_{n,7,k}(1) = f_{n,8,k}(0), \quad f'_{n,7,k}(1) = f'_{n,8,k}(0), \\ f_{n,8,k}(1) = f_{n,9,k}(0), \quad f'_{n,8,k}(1) = f'_{n,9,k}(0) \end{array} \right\}.$$

for  $n \in \mathbb{Z}$  and  $k \in \mathbb{Z}_N$



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

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

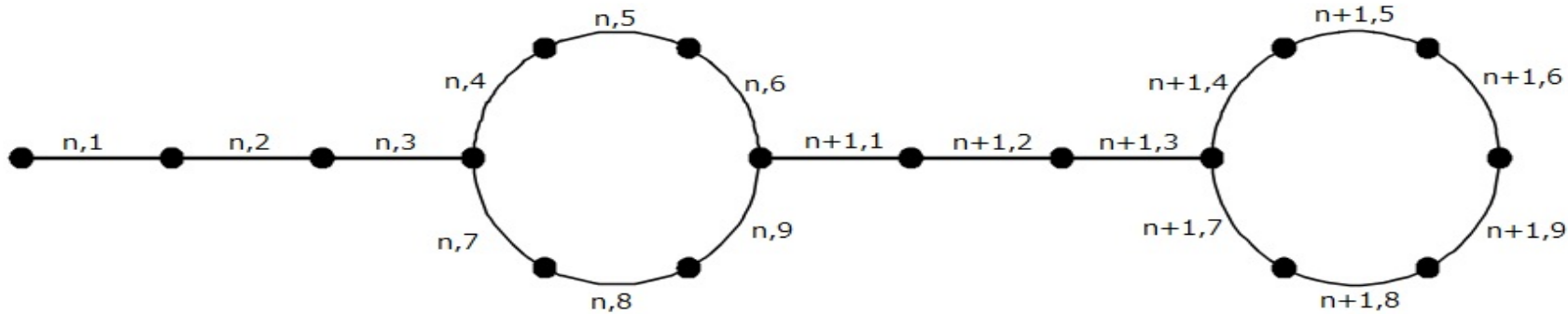


Fig. 6 A degenerate zigzag supergraphene-based CNT  $\Gamma^1$ .

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

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

Dom( $H_k$ )

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

- 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

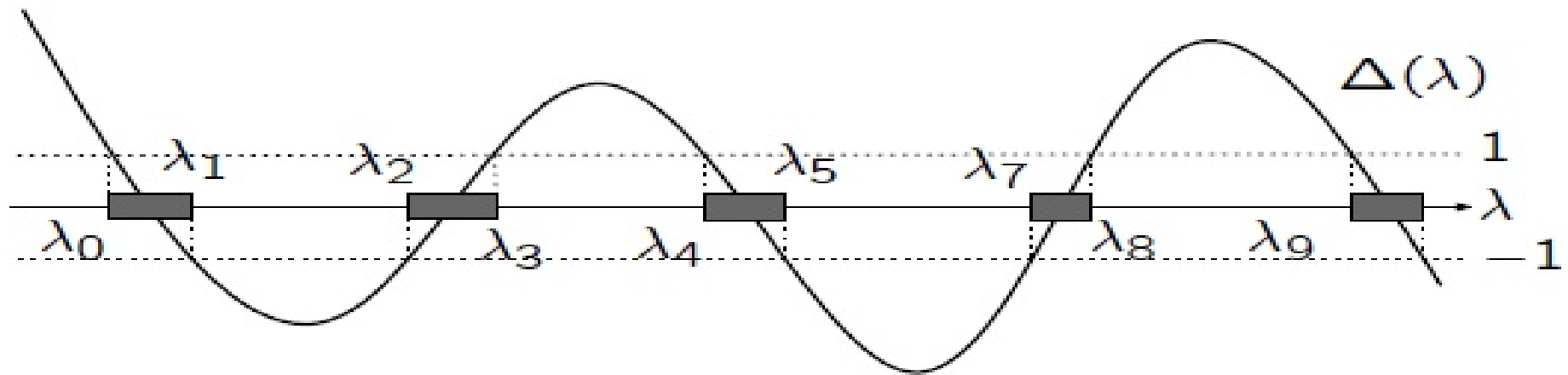
$$-y''(x, \lambda) + q(x)y(x, \lambda) = \lambda y(x, \lambda), \quad x \in \mathbb{R}, \quad (1)$$

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

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

where  $\lambda_0, \lambda_1, \lambda_2, \dots$  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  $j$ 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 called the  $j$ th 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)  $\sigma_{1/2}(L) := \{\lambda \in \mathbb{R} \mid \Delta = \frac{1}{2}\}$ .  
 $\sigma_{-1/2}(L) := \{\lambda \in \mathbb{R} \mid \Delta = -\frac{1}{2}\}$ .  
 $\sigma_{\pm 1/2}(L) := \sigma_{1/2}(L) \cup \sigma_{-1/2}(L)$ .

## 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

$$\begin{aligned} D(\ell, \lambda) &= D\left(\frac{N}{2}, \lambda\right) \\ &= 144\Delta_-^6 - (216 + 16\Delta_-^2)\Delta_-^4 + (81 + 8\Delta_-^2)\Delta_-^2 - (1 + \Delta_-^2) \end{aligned}$$

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

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

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

For  $k = 1, 2, \dots, N$ , 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:



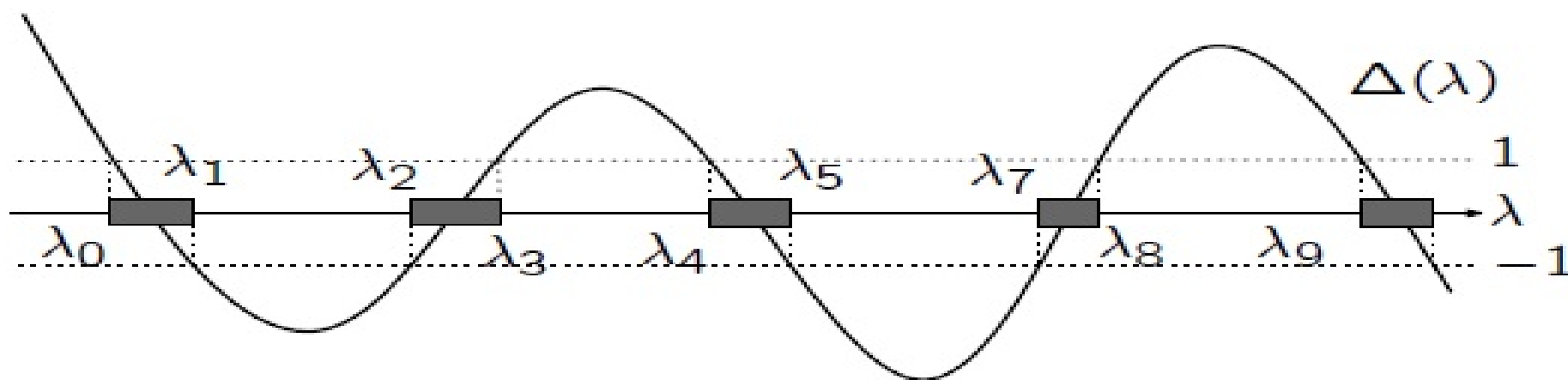
**Theorem 2.1.** For a fixed  $\ell \in \mathbb{N}$ , we obtain the followings:

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

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

and

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



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

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

and

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

Abbreviate  $\theta(1, \lambda)$ ,  $\theta'(1, \lambda)$ ,  $\varphi(1, \lambda)$ ,  $\varphi'(1, \lambda)$  to  $\theta_1$ ,  $\theta'_1$ ,  $\varphi_1$ ,  $\varphi'_1$ .

**Lemma 2.2.** *For a fixed  $N \in \mathbb{N}$ , we have*

$$\sigma_{1/2}(L) \cup \sigma_{-1/2}(L) \subset \sigma_{\infty}(H_k) \text{ for } k = 1, 2, \dots, N.$$

*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

$$u_{0,4}^{(0)}(x, \lambda) = \varphi(x, \lambda), \quad u_{0,5}^{(0)}(x, \lambda) = v_1(x, \lambda),$$

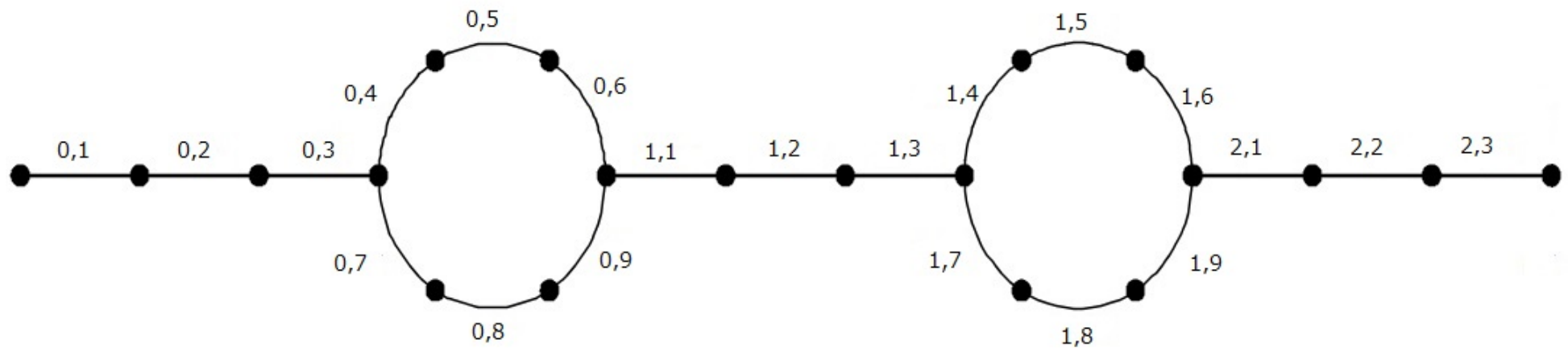
$$u_{0,6}^{(0)}(x, \lambda) = v_2(x, \lambda), \quad u_{0,7}^{(0)}(x, \lambda) = -\varphi(x, \lambda),$$

$$u_{0,8}^{(0)}(x, \lambda) = -v_1(x, \lambda), \quad u_{0,9}^{(0)}(x, \lambda) = -v_2(x, \lambda)$$

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  $u^{(n)} = \{u_{m-n,j}^{(0)}\}_{(m,j) \in \mathcal{Z}_1}$ . Then, we can directly check  $\{u^{(n)}\}_{n \in \mathbb{Z}} \subset \text{Dom}(H_0)$  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  $k = 1, 2, \dots, N - 1$ . Then, we put

$$\alpha_k = -1 + s^{-k}, \quad \beta_k = \frac{1-s^{-k}}{1-s^k}, \quad \gamma_k = -\frac{1-s^{-k}}{1-s^k},$$

$$u_{0,4}^{(0)}(x, \lambda) = \varphi(x, \lambda), \quad u_{0,5}^{(0)}(x, \lambda) = v_1(x, \lambda),$$

$$u_{0,6}^{(0)}(x, \lambda) = v_2(x, \lambda), \quad u_{0,7}^{(0)}(x, \lambda) = -s^{-k}\varphi(x, \lambda),$$

$$u_{0,8}^{(0)}(x, \lambda) = -s^{-k}v_1(x, \lambda), \quad u_{0,9}^{(0)}(x, \lambda) = -s^{-k}v_2(x, \lambda),$$

$$u_{1,1}(x, \lambda) = \alpha_k\varphi(x, \lambda), \quad u_{1,2}(x, \lambda) = \alpha_kv_1(x, \lambda),$$

$$u_{1,3}(x, \lambda) = \alpha_kv_2(x, \lambda), \quad u_{1,4}(x, \lambda) = \beta_k\varphi(x, \lambda),$$

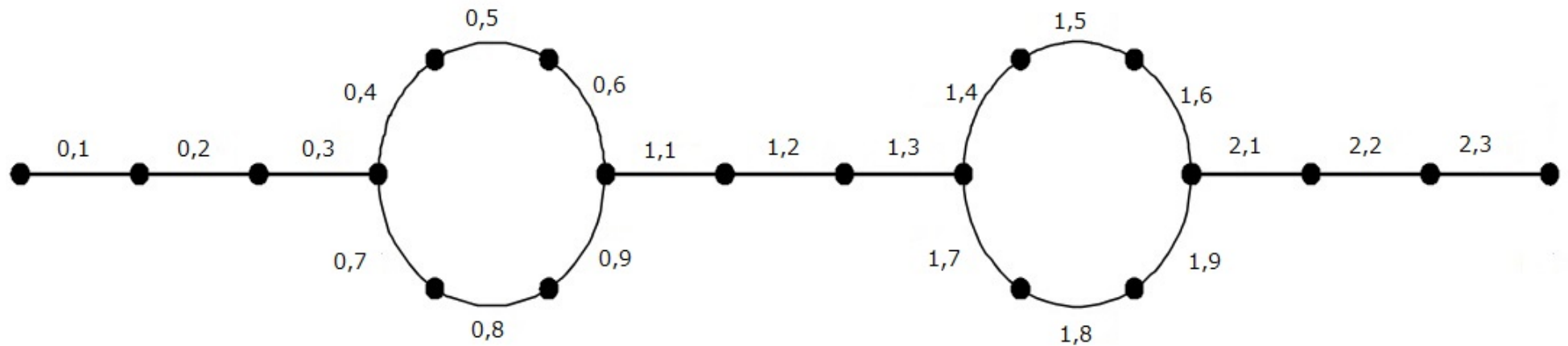
$$u_{1,5}(x, \lambda) = \beta_kv_1(x, \lambda), \quad u_{1,6}(x, \lambda) = \beta_kv_2(x, \lambda),$$

$$u_{1,7}(x, \lambda) = \gamma_k\varphi(x, \lambda), \quad u_{1,8}(x, \lambda) = \gamma_kv_1(x, \lambda),$$

$$u_{1,9}(x, \lambda) = \gamma_kv_2(x, \lambda).$$

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  $\lambda \in \sigma_{-1/2}(L)$ . □

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

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

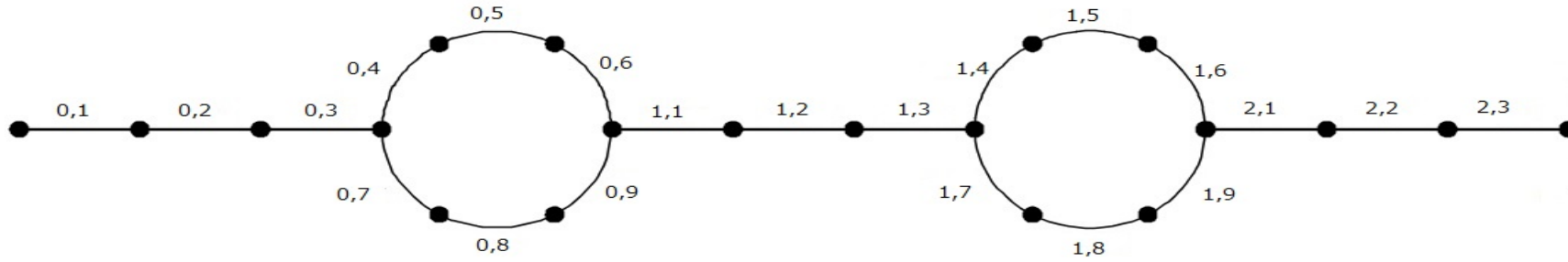
$\mathcal{H}_\mu = \bigoplus_{j=1}^9 L^2(\Gamma_{0,j})$ . Prepare the Hilbert space

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

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

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

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



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

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



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  $\lambda$ , we consider the characteristic equation  $H_k(\mu)f = \lambda f$  for  $0 \neq f = (f_j)_{j=1}^9 \in \text{Dom}(H_k(\mu))$ . Namely, we consider the following system:

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

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

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

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

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

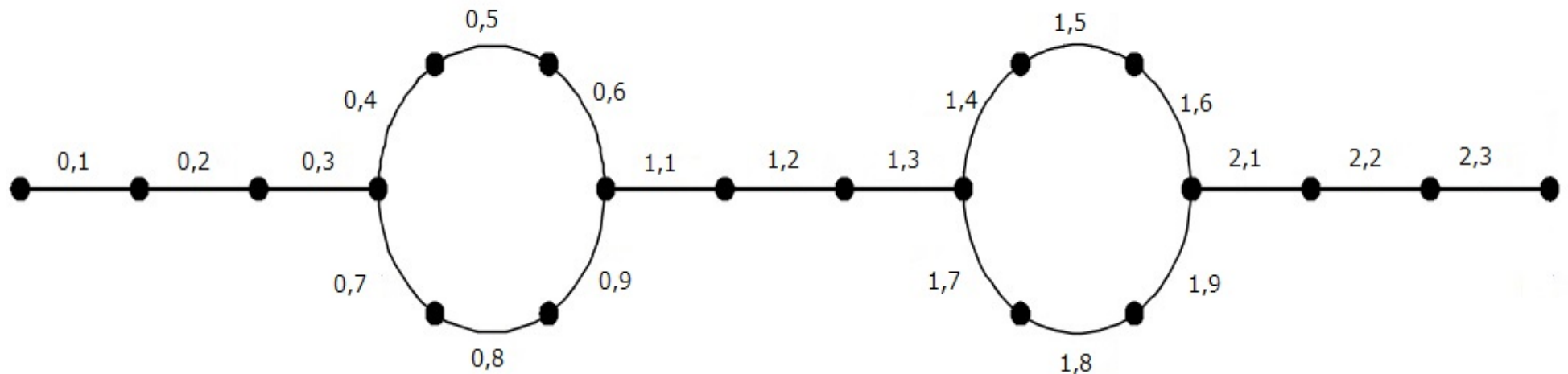
$$f_5'(1) = f_6'(0), \quad f_7'(1) = f_8'(0), \quad f_8'(1) = f_9'(0), \quad (8)$$

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

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

$$\begin{aligned}
 f_1(x, \lambda) &= w(x, \lambda) X_1 + \frac{\varphi(x, \lambda)}{\varphi_1} X_2, & f_2(x, \lambda) &= w(x, \lambda) X_2 + \frac{\varphi(x, \lambda)}{\varphi_1} X_3, \\
 f_3(x, \lambda) &= w(x, \lambda) X_3 + \frac{\varphi(x, \lambda)}{\varphi_1} X_4, & f_4(x, \lambda) &= w(x, \lambda) X_4 + \frac{\varphi(x, \lambda)}{\varphi_1} X_5, \\
 f_5(x, \lambda) &= w(x, \lambda) X_5 + \frac{\varphi(x, \lambda)}{\varphi_1} X_6, & f_6(x, \lambda) &= w(x, \lambda) X_6 + \frac{\varphi(x, \lambda)}{\varphi_1} e^{i\mu} X_1, \\
 f_7(x, \lambda) &= w(x, \lambda) X_4 + \frac{\varphi(x, \lambda)}{\varphi_1} X_7, & f_8(x, \lambda) &= w(x, \lambda) X_7 + \frac{\varphi(x, \lambda)}{\varphi_1} X_8, \\
 f_9(x, \lambda) &= w(x, \lambda) X_8 + \frac{\varphi(x, \lambda)}{\varphi_1} e^{i\mu} X_1
 \end{aligned}$$

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:

$$X_1 - 2\Delta X_2 + X_3 = 0,$$

$$X_2 - 2\Delta X_3 + X_4 = 0,$$

$$X_3 - (2\theta_1 + \varphi'_1)X_4 + X_5 + s^k X_7 = 0,$$

$$X_4 - 2\Delta X_5 + X_6 = 0,$$

$$e^{i\mu} X_1 + X_5 - 2\Delta X_6 = 0,$$

$$s^{-k} X_4 - 2\Delta X_7 + X_8 = 0,$$

$$e^{i\mu} X_1 + X_7 - 2\Delta X_8 = 0,$$

$$-(2\varphi'_1 + \theta_1)e^{i\mu} X_1 + e^{i\mu} X_2 + X_6 + X_8 = 0.$$

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  $X_1, X_2, \dots, X_8$ :

$$\begin{pmatrix} 1 & -2\Delta & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & -2\Delta & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & -(2\theta_1 + \varphi'_1) & 1 & 0 & s^k & 0 \\ 0 & 0 & 0 & 1 & -2\Delta & 1 & 0 & 0 \\ e^{i\mu} & 0 & 0 & 0 & 1 & -2\Delta & 0 & 0 \\ 0 & 0 & 0 & s^{-k} & 0 & 0 & -2\Delta & 1 \\ e^{i\mu} & 0 & 0 & 0 & 0 & 0 & 1 & -2\Delta \\ -(2\varphi'_1 + \theta_1)e^{i\mu} & e^{i\mu} & 0 & 0 & 0 & 1 & 0 & 1 \end{pmatrix}.$$

We have a dispersion relation

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

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

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

### 3 Absolutely continuous spectrum of $H_k$ : Unperturbed case

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



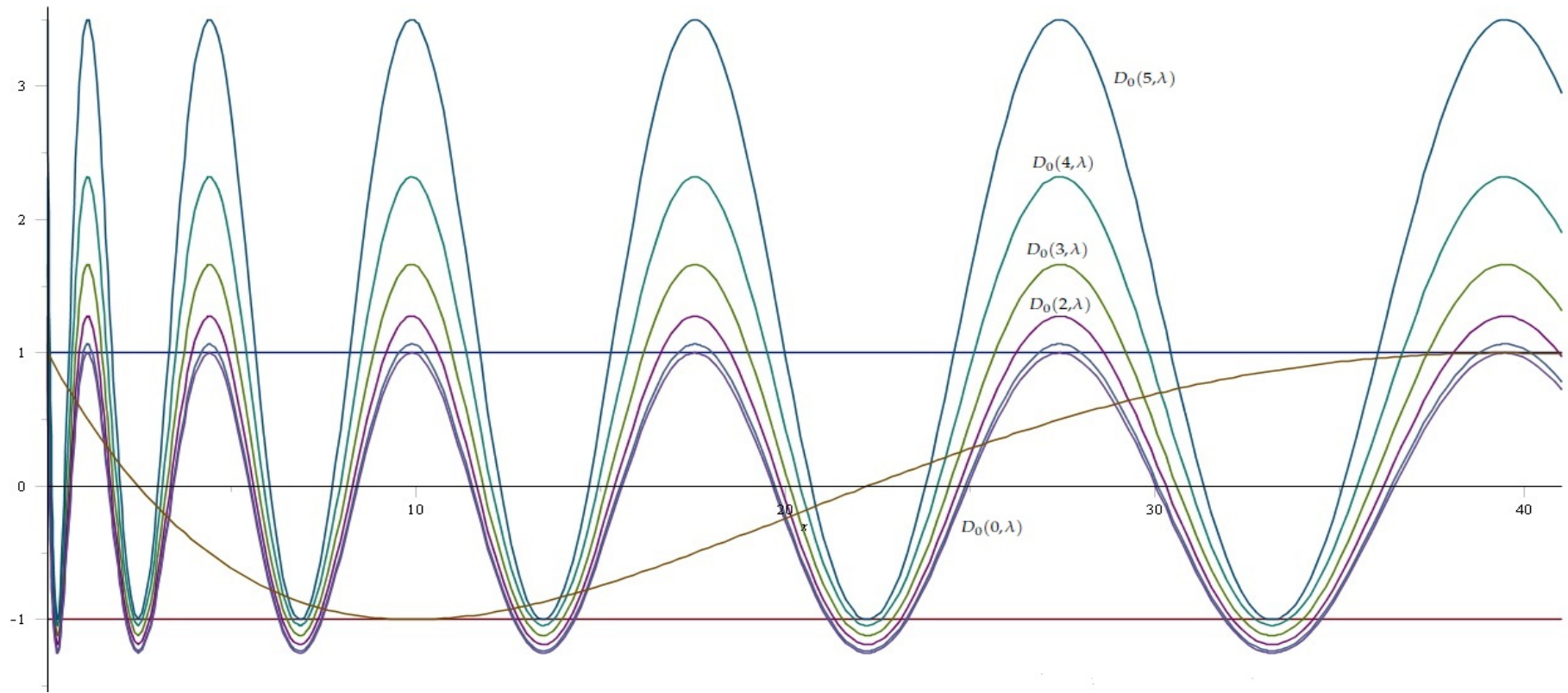


Fig. 7 The graph of  $D_0(0, \lambda)$ ,  $D_0(1, \lambda)$ ,  $D_0(2, \lambda)$ ,  $D_0(3, \lambda)$ ,  $D_0(4, \lambda)$ ,  $D_0(5, \lambda)$  and  $\cos \sqrt{\lambda}$  in the case where  $N = 15$ . This picture hinted the results of the following Theorem 4.1. Namely, one can numerically expect that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

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**Theorem 4.1.** *Let  $N = 2\ell - 1$  or  $N = 2\ell$  for a fixed  $\ell \in \mathbb{N}$ .*

*(i) For  $k = 0, 1, 2, \dots, N$ , 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  $k = 0, 1, 2, \dots, \ell - 1$ , there exists real sequence*

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

*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  $\sigma_{k,j} = [\lambda_{k,j-1}^+, \lambda_{k,j}^-]$  and the  $j$ th 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

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

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

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

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

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

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

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

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

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

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

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

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

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

**Theorem 4.2.** (i) *Edges of even-numbered spectral gaps behave as follows:*

(a) *Let  $k = 1, 2, \dots, \ell - 1$ . For  $p = 1, 2, 3, 4, 5, 6$ , we have*

$$\lambda_{k,12n+2p}^{\pm} = (u_{k,12n+2p}^{\pm})^2 + q_0 + o\left(\frac{1}{n}\right) \quad \text{as } n \rightarrow \infty.$$

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

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

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

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

*as  $n \rightarrow \infty$ .*

(ii) Edges of odd-numbered 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

$$\lambda_{k,12n+p}^{\pm} = (u_{k,12n+p}^{\pm})^2 + q_0 + o\left(\frac{1}{n}\right) \quad \text{as } n \rightarrow \infty.$$

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

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

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

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

as  $n \rightarrow \infty$ .

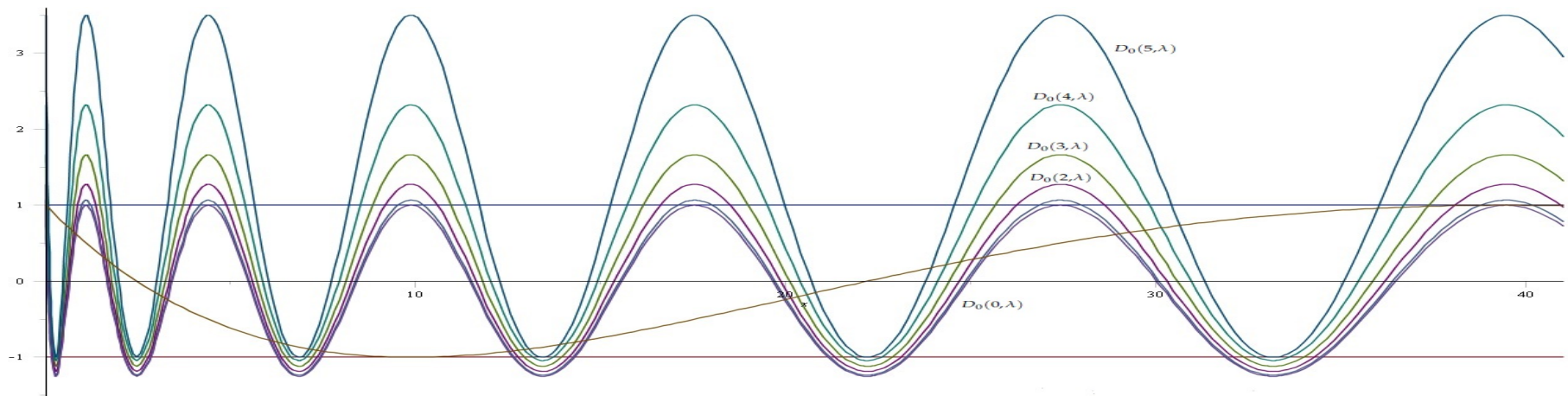
## Absence of spectral gaps

**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  $k = 0, 1, \dots, \ell - 1$ .

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

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

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  $k = 0, 1, \dots, \ell - 1$ , there exists some  $\lambda_0 \in \mathbb{R}$  such that

$$D_k^- > 0 \text{ for any } \lambda \geq \lambda_0.$$

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  $\lambda \rightarrow +\infty$ .

To be continued in ...

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

Thank you for your attention.

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