Schrödinger operators on armchair nanotubes. II

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Abstract

We consider the Schrödinger operator with a periodic potential on quasi-1D models of armchair single-wall nanotubes. The spectrum of this operator consists of an absolutely continuous part (intervals separated by gaps) plus an infinite number of eigenvalues with infinite multiplicity. We describe the absolutely continuous spectrum of the Schrödinger operator: 1) the multiplicity, 2) endpoints of the gaps, they are given by periodic or antiperiodic eigenvalues or resonances (branch points of the Lyapunov function), 3) resonance gaps, where the Lyapunov function is non-real. We determine the asymptotics of the gaps at high energy.

1 Introduction and main results

Consider the Schrödinger operator $\mathcal{H} = -\Delta + \mathcal{V}_q$ with a periodic potential $\mathcal{V}_q$ on so called armchair graph $\Gamma_N$, $N \geq 1$. In order to describe the graph $\Gamma_N$, we introduce the fundamental cell $\overline{\Gamma} = \bigcup_i \overline{\Gamma}_j \subset \mathbb{R}^2$, where $\overline{\Gamma}_j = \{x = \tilde{r}_j + te_j, t \in [0,1], j \in \mathbb{N}_6$ is the edge of length 1, and

$$N_m = \{1, 2, ..., m\}, \quad e_1 = e_6 = \frac{1}{2}(1, \sqrt{3}), \quad e_2 = e_4 = (1, 0), \quad e_3 = -e_5 = \frac{1}{2}(1, -\sqrt{3}),$$

$$\tilde{r}_1 = (0, 0), \quad \tilde{r}_2 = \tilde{r}_5 = \tilde{r}_1 + e_1, \quad \tilde{r}_3 = \tilde{r}_6 = \tilde{r}_2 + e_2, \quad \tilde{r}_4 = \tilde{r}_3 + e_3. \quad (1.1)$$

We define the strip graph $\overline{\Gamma}^N$ by

$$\overline{\Gamma}^N = \bigcup_{(n,k) \in \mathbb{Z} \times \mathbb{N}_N} (\overline{\Gamma} + ke_h + ne_v) \subset \mathbb{R}^2, \quad e_h = (3, 0), \quad e_v = (0, \sqrt{3}).$$

Vertices of $\overline{\Gamma}^N$ are $\tilde{r}_j + ke_h + ne_v$, $(n, j, k) \in \mathbb{Z} \times \mathbb{N}_6 \times \mathbb{N}_N$. If we identify the vertices $\tilde{r}_1 + ne_v$ and $\tilde{r}_1 + Ne_h + ne_v$ of $\overline{\Gamma}^N$ for each $n \in \mathbb{Z}$, then we obtain the graph $\Gamma^N$, given by

$$\Gamma^N = \bigcup_{\omega \in \mathbb{Z}} \Gamma^N, \quad \omega = (n, j, k) \in \mathbb{Z} = \mathbb{Z} \times \mathbb{N}_6 \times \mathbb{Z}_N, \quad \mathbb{Z}_N = \mathbb{Z}/(N\mathbb{Z}).$$

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where $\Gamma_\omega = \tilde{\Gamma}_j + ke^h + ne^v$, see Fig. 1. Let $r_\omega = \tilde{r}_j + ke^h + ne^v$ be a starting point of the edge $\Gamma_\omega$. We have the coordinate $x = r_\omega + te^j$ and the local coordinate $t \in [0, 1]$ on $\Gamma_\omega$. Thus we give an orientation on the edge. For each function $y$ on $\Gamma^N$ we define a function $y_\omega = \tilde{y}_j + ke^h + ne^v$ be a starting point of the edge $\Gamma_\omega$. W e have the coordinate $x = r_\omega + te^j$ and the local coordinate $t \in [0, 1]$ on $\Gamma_\omega$. W e have the coordinate $x = r_\omega + te^j$ and the local coordinate $t \in [0, 1]$ on $\Gamma_\omega$.

**Kirchhoff Boundary Conditions:** $y \in C(\Gamma^N)$ satisfies for each vertex $A$ of $\Gamma^N$

\[
\sum_{\omega \in E_A} (-1)^b y'_\omega (b) = 0, \quad \text{where} \quad E_A = \{\omega \in \mathcal{Z} : A \in \Gamma_\omega\}, \quad b = b(\omega, A), \tag{1.2}
\]

where if $A = r_\omega$ is a starting point of $\Gamma_\omega$ (i.e. $t = 0$ at $A$), then $b(\omega, A) = 0$,

if $A = r_\omega + e^j$ is an endpoint of $\Gamma_\omega$ (i.e. $t = 1$ at $A$), then $b(\omega, A) = 1$.

The Kirchhoff Conditions (1.2) mean that the sum of derivatives of $y$ at each vertex of $\Gamma^N$ equals 0 and the orientation of edges gives the sign ±. Our operator $\mathcal{H}$ on $\Gamma^N$ acts in the Hilbert space $L^2(\Gamma^N)$ and is given by $(\mathcal{H}y)_\omega = -y''_\omega + qy_\omega$, where $y = (y_\omega)_{\omega \in \mathcal{Z}} \in \mathcal{D}(\mathcal{H}) = W^2(\Gamma^N)$ and $(\mathcal{H}q)_\omega = qy_\omega, q \in L^2(0, 1)$. If the potential $q$ is **even**, i.e., $q \in L^2_{\text{even}}(0, 1) = \{q \in L^2(0, 1) : q(t) = q(1-t), t \in [0, 1]\}$, then the orientation of edges is not important. The standard arguments (see [KL]) yield that $\mathcal{H}$ is self-adjoint.

The considered model was introduced by Pauling [Pa] and was systematically developed in the series of articles by Ruedenberg and Scherr [RS]. Further progress is discussed in [KL, KLI, BBKL, Ha, SDD] and see references therein.
Figure 2: A piece of a nanotube $\Gamma^N$. The fundamental domain is marked by a bold line.

For the convenience of the reader we briefly describe the structure of carbon nanotubes, see [Ha, SDD]. Graphene is a single 2D layer of graphite forming a honeycomb lattice, see Fig. 3. A carbon nanotube is a honeycomb lattice "rolled up" into a cylinder, see Fig. 1. In carbon nanotubes, the graphene sheet is "rolled up" in such a way that the so-called chiral vector $\Omega = N_1\Omega_1 + N_2\Omega_2$ becomes the circumference of the tube, where $\Omega_1, \Omega_2$ are defined in Fig. 3. The chiral vector $\Omega$, which is usually denoted by the pair of integers $(N_1, N_2)$, uniquely defines a particular tube. Tubes of type $(N, 0)$ are called zigzag tubes. $(N, N)$-tubes are called armchair tubes.

Recall the needed properties of the Hill operator $\tilde{Hy} = -y'' + q(t)y$ on the real line with a periodic potential $q(t + 1) = q(t), t \in \mathbb{R}$. The spectrum of $\tilde{H}$ is purely absolutely continuous and consists of intervals $\tilde{\sigma}_n = [\tilde{\lambda}_{n-1}^+, \tilde{\lambda}_n^-], n \geq 1$. These intervals are separated by the gaps $\tilde{\gamma}_n = (\tilde{\lambda}_n^-, \tilde{\lambda}_n^+)$ of length $|\tilde{\gamma}_n| \geq 0$. If a gap $\tilde{\gamma}_n$ is degenerate, i.e. $|\tilde{\gamma}_n| = 0$, then the corresponding segments $\tilde{\sigma}_n, \tilde{\sigma}_{n+1}$ merge. For the equation $-y'' + q(t)y = \lambda y$ on the real line we define the fundamental solutions $\vartheta(t, \lambda)$ and $\varphi(t, \lambda), t \in \mathbb{R}$ satisfying $\vartheta(0, \lambda) = \varphi'(0, \lambda) = 1, \vartheta'(0, \lambda) = \varphi(0, \lambda) = 0$. We define the monodromy matrix $\tilde{M}$, the Lyapunov function $F$, and the function $F_-$ by

$$
\tilde{M} = \begin{pmatrix} \vartheta_1 & \varphi_1 \\ \varphi'_1 & \varphi_1 \end{pmatrix}, \quad F = \frac{\varphi'_1 + \vartheta_1}{2}, \quad F_- = \frac{\varphi'_1 - \vartheta_1}{2},
$$

where $\varphi_1 = \varphi(1, \cdot), \vartheta_1 = \vartheta(1, \cdot), \varphi'_1 = \varphi'(1, \cdot), \vartheta'_1 = \vartheta'(1, \cdot)$. The function $F$ has only simple zeros $\eta_n, n \geq 1$, which satisfy $\eta_1 < \eta_2 < \ldots$. The sequence $\tilde{\lambda}_0^+ < \tilde{\lambda}_1^- < \ldots$ is the spectrum of the equation $-y'' + qy = \lambda y$ with 2-periodic boundary conditions, that is $y(t + 2) = y(t), t \in \mathbb{R}$. Here equality $\tilde{\lambda}_n^- = \tilde{\lambda}_n^+$ means that $\tilde{\lambda}_n^\pm$ is an eigenvalue of multiplicity 2. Note
that $F(\tilde{\lambda}_n^\pm) = (-1)^n$, $n \geq 1$. The lowest eigenvalue $\tilde{\lambda}_0^\pm$ is simple, $F(\tilde{\lambda}_0^+) = 1$, and the corresponding eigenfunction has period 1. The eigenfunctions corresponding to period 1 if $n$ is odd. The derivative of the Lyapunov function has a zero

$$F$$

$$N$$

$$\Omega = \tilde{\lambda}_n^\pm$$ have period 1 if $n$ is even, and they are anti-periodic, that is $y(t + 1) = -y(t)$, $t \in \mathbb{R}$, if $n$ is odd. The derivative of the Lyapunov function has a zero $F'\tilde{\lambda}_n = 0$. Let $\mu_n, n \geq 1$, be the spectrum of the problem $-y'' + qy = \lambda y$, $y(0) = y(1) = 0$ (the Dirichlet spectrum). Define the set $\sigma_D = \{\mu_n, n \geq 1\}$ and note that $\sigma_D = \{\lambda \in \mathbb{C} : \varphi(1, \lambda) = 0\}$. It is well-known that $\mu_n \in [\tilde{\lambda}_n^-, \tilde{\lambda}_n^+], n \geq 1$.

For simplicity we shall denote $\Gamma_{n,1} \subset \Gamma^1$ by $\Gamma_\alpha$, for $\alpha = (n,j) \in \mathbb{Z}_1 = \mathbb{Z} \times \mathbb{N}_0$. Thus $\Gamma^1 = \bigcup_{\alpha \in \mathbb{Z}_1} \Gamma_\alpha$, see Fig 1. We introduce the self adjoint operator $H_k$ acting in the Hilbert space $L^2(\Gamma^1)$ and given by $(H_k f)_\alpha = -f''_\alpha + qf_\alpha, (f_\alpha)_{\alpha \in \mathbb{Z}_1}, (f''_\alpha)_{\alpha \in \mathbb{Z}_1} \in L^2(\Gamma^1)$, where the components $f_\alpha, \alpha \in \mathbb{Z}_1$ satisfy the Kirchhoff conditions:

$$f_{n,1}(1) = f_{n,2}(0) = f_{n,5}(0), \quad f_{n,2}(1) = f_{n,3}(0) = f_{n,6}(0),$$

$$f_{n,3}(1) = f_{n,4}(0) = f_{n-1,6}(1), \quad s^kf_{n,4}(1) = f_{n,1}(0) = f_{n-1,5}(1), \quad s = e^{\pm i \pi N}.$$

$$f'_{n,1}(1) - f'_{n,2}(0) - f'_{n,5}(0) = 0, \quad f'_{n,2}(1) - f'_{n,3}(0) - f'_{n,6}(0) = 0,$$

$$f'_{n,3}(1) - f'_{n,4}(0) + f'_{n-1,6}(1) = 0, \quad s^kf'_{n,4}(1) - f'_{n,1}(0) + f'_{n-1,5}(1) = 0.$$

The operator $H_k$ has four Floquet solutions $\psi_{k,\nu}^{\mu, \pm} = (\psi_{k,\alpha}^{\mu, \pm})_{\alpha \in \mathbb{Z}_1}, \nu = 1, 2$ satisfying the condition

$$\begin{pmatrix}
\psi_{k,1,5}^{\mu, \pm}(1) \\
\psi_{k,1,6}^{\mu, \pm}(1)
\end{pmatrix} = \tau_{k,\nu}^{\pm} \begin{pmatrix}
\psi_{k,0,5}^{\mu, \pm}(1) \\
\psi_{k,0,6}^{\mu, \pm}(1)
\end{pmatrix}.$$
The operator $\mathcal{H}$ is unitarily equivalent to $H = \bigoplus_1^N H_k$. The following identities hold true:

$$\sigma(H_k) = \sigma_{\text{ac}}(H_k), \quad \sigma_{\text{ac}}(H_k) = \sigma_D,$$

$$\sigma_{\text{ac}}(H_k) = \{ \lambda \in \mathbb{R} : F_{k,\nu}(\lambda) \in [-1, 1] \text{ for some } \nu \in \mathbb{N}_2 \}, \quad (1.6)$$

$$F_{k,\nu} = \xi_k - (-1)^\nu \sqrt{\rho_k}, \quad \nu = 1, 2, \quad \xi_k = \frac{9F^2 - F^2 - 1}{2}, \quad \rho_k = (9F^2 - s_k^2) c_k + s_k^2 F^2 \quad (1.7)$$

for each $k \in \mathbb{Z}_N$, where $s_k = \sin \frac{\pi k}{N}$, $c_k = \cos \frac{\pi k}{N}$. Here the functions $F_{k,1}, F_{k,2}$ are branches of the Lyapunov functions $F_k = \xi_k + \sqrt{\rho_k}$, analytic on the two-sheeted Riemann surface $\mathcal{R}_k$ defined by $\sqrt{\rho_k}$.

**Remark.** We take the branch of $\sqrt{\rho_k}$ such that $\sqrt{\rho_k(\lambda)} > 0$, where $\rho_k(\lambda) > 0, \lambda \in \mathbb{R}$. Then $F_{k,1} = \xi_k + \sqrt{\rho_k} > F_{k,2} = \xi_k - \sqrt{\rho_k}$ for such $\lambda$. Note that $F_{k,\nu}, k \notin \{0, \frac{N}{2}\}$ have branch points on the real line. The functions $F_{0,\nu}', \nu = 1, 2$ have steps at the points $\pm n, n \geq 1$. The functions $F_{m,\nu}', m = \frac{N}{2} \in \mathbb{Z}$ have steps at the zeros of $F_-$. Note that using other branches of $\sqrt{\rho_k}$ we could obtain a new smooth functions $F_{k,\nu}$ on real axis for $k \in \{0, \frac{N}{2}\}$, but this choice is not convenient for our proof.

We define the entire functions

$$D_k^\pm = 4(F_{k,1} \mp 1)(F_{k,2} \mp 1). \quad (1.8)$$

The zeros $\lambda_{\nu,2n}^k, n \geq 0, \nu = 1, 2$, of the function $D_k^+$ are the periodic eigenvalues. The zeros $\lambda_{\nu,2n-1}^k, n \geq 1, \nu = 1, 2$, of $D_k^-$ are the antiperiodic eigenvalues. Let $\lambda_{2,0}^k \leq \lambda_{1,0}^k \leq \lambda_{1,2}^k \leq \lambda_{2,2}^k \leq \lambda_{2,1}^k \leq \lambda_{1,1}^k \leq \lambda_{2,3}^k \leq \lambda_{1,3}^k \leq \ldots$ counted with multiplicities. This labeling is convenient for us and associated with the Lyapunov functions $F_{k,1}, F_{k,2}$ (see Fig 1).

A zero of $\rho_k, k \in \mathbb{Z}_N$ is called a resonance of $H_k$. Roughly speaking the simple real resonances create gaps. There exist real and non-real resonances for $k \notin \{0, \frac{N}{2}\}$ (see [BBKL]). Note that in the case of zigzag nanotube all resonances are real [KL], [KLI].

We define the functions

$$u_k = |F_-| - s_k^2, \quad v_k = |F_-| - c_k^2, \quad k \in \mathbb{Z}_N. \quad (1.9)$$

**Theorem 1.1.** Let $k \in \mathbb{Z}_N$. Then the identity $\sigma_{\text{ac}}(H_k) = \bigcup_{\nu \in \mathbb{N}_2, n \geq 1} S_{\nu,n}^k$ holds, where the spectral bands $S_{\nu,n}^k = [E_{\nu,n}^{k,+}, E_{\nu,n}^{k,-}], \nu = 1, 2, n \geq 1$ satisfy:

$$E_{\nu,n}^{k,+} = \lambda_{\nu,n}^{k,+}, \quad E_{\nu,n}^{k,-} = \lambda_{\nu,n}^{k,-}, \quad E_{1,p}^{k,\pm} = \begin{cases} \lambda_{1,p}^{0,\pm} & \text{if } v_k(\lambda_{1,p}^{0,\pm}) \geq 0 \\ r_{k,n}^\pm & \text{if } v_k(\lambda_{1,p}^{0,\pm}) < 0 \end{cases}, \quad p = 2n - 1, \quad (1.10)$$

$$E_{1,p}^{k,\pm} = r_{k,n}^\pm \text{ for } k \notin \{0, \frac{N}{2}\} \text{ and for large } n \geq 1, \text{ where } r_{k,n}^\pm \text{ are given by}$$

$$r_{k,n}^- = \min \{ \lambda \in \mathbb{R}_n : \rho_k(\lambda) = 0 \}, \quad r_{k,n}^+ = \max \{ \lambda \in \mathbb{R}_n : \rho_k(\lambda) = 0 \}, \quad \mathcal{R}_n = (\lambda_{1,p}^{0,-}, \lambda_{1,p}^{0,+}).$$
Moreover, the following estimates hold true:

\[ E_{2p-1}^{k,+} \leq \min\{E_{2p}^{k,-}, E_{1p}^{k,+}\} \leq \max\{E_{2p}^{k,-}, E_{1p-1}^{k,+}\} \leq E_{1p}^{k,-} \]
\[ \leq E_{1p}^{k,+} \leq \min\{E_{1p+1}^{k,-}, E_{2p}^{k,+}\} \leq \max\{E_{1p+1}^{k,-}, E_{2p}^{k,+}\} \leq E_{2p+1}^{k,-}. \quad (1.11) \]

\[ E_{2p}^{k,-} > E_{1p-1}^{k,+} \text{ iff } u_k(E_{2p}^{k,-}) < 0; \quad E_{1p+1}^{k,-} > E_{2p}^{k,+} \text{ iff } u_k(E_{2p}^{k,+}) < 0. \quad (1.12) \]

**Remark.** (i) The second identity in (1.10) shows that \( E_{2p}^{k,\pm} = E_{2p}^{0,\pm} \) for all \((k,n) \in \mathbb{Z}_N \times \mathbb{N}\). Here and below \( p = 2n - 1 \).

(ii) The last identity in (1.7) gives \( \rho_0 = 9F^2 \) and then \( r_{0n}^\pm = \eta_n \) are zeros of \( F \).

(iii) Let \( k \neq \frac{N}{2} \). If \( v_k(\lambda_{0p}^\sigma) < 0 \) for some \( \sigma = \pm \), then \( \rho_k \) has at least two zeros \( r_{k,n}^\pm \) in \( \mathbb{R}_+ \), (see Lemma 3.2(iii)). In Lemma 3.4 we prove that the last identity in (1.10) for \( k \neq \frac{N}{2} \) is equivalent to

\[ E_{1p}^{k,\pm} = \begin{cases} 
\lambda_{1p}^{0,\pm} & \text{if } F_{k,1}(r_{k,n}^\pm) = F_{k,2}(r_{k,n}^\pm) \leq -1 \text{ or } \rho_k > 0 \text{ on } \mathbb{R}_n \n\rho_{k,n}^\pm & \text{if } F_{k,1}(r_{k,n}^\pm) = F_{k,2}(r_{k,n}^\pm) \in (-1, \frac{1}{2}] \end{cases}, \quad k \neq \frac{N}{2}. \]

(iv) Let \( k = m = \frac{N}{2} \in \mathbb{Z} \). Then \( c_m = 0 \) and (1.7) gives \( \rho_m = F^2 \). Thus, \( v_m = |F_-| \) and \( v_m(\lambda_{1p}^{0,\pm}) \geq 0 \) for all \( n \geq 1 \), where \( p = 2n - 1 \). The last identity in (1.10) gives \( E_{1p}^{m,\pm} = \lambda_{1p}^{0,\pm} \).

**Theorem 1.2.** Let \( k \in \mathbb{Z}_N, n \geq 1, p = 2n - 1 \).

(i) Let \( \mathbb{R}_{k,n}^- = (\lambda_{1p}^{0,-}, r_{k,n}^-) \subset S_{k,2n-1}^k, \mathbb{R}_{k,n}^+ = (r_{k,n}^+, \lambda_{1p}^{0,+}) \subset S_{k,2n}^k \) (i.e., \( E_{1p}^{k,\pm} = r_{k,n}^\pm \)). Then the spectrum of \( H_k \) in \( \mathbb{R}_{k,n}^+ \neq \emptyset \) has multiplicity 4.
(ii) If $E_{2,p}^{k,-} > E_{1,p-1}^{k,+}$ (or $E_{1,p+1}^{k,-} > E_{2,p}^{k,+}$), then the spectrum of $H_k$ in the interval $(E_{1,p-1}^{k,+}, E_{2,p}^{k,-}) = S_{1,p}^k \cap S_{2,p}^k$ (or $(E_{2,p}^{k,+}, E_{1,p-1}^{k,-}) = S_{1,p+1}^k \cap S_{2,p}^k$) has multiplicity 4.

(iii) The spectrum $\sigma_{ac}(H_k)$ in all intervals, with the exception the intervals of the statements (i), (ii), has multiplicity 2.

**Remark** (i) Let $q \in L^2_{even}(0,1)$. In this case $F_- = 0$ (see p.8, [MW]). If $k \neq 1/2$, then $v_k(\lambda_{1,p}^{0,\pm}) = -c^2_k < 0$ and the last identity in (1.10) gives $E_{1,p}^{k,\pm} = \gamma_{k,n}$ for all $n \geq 1$. If $k \neq 0$, then $u_k = -s_k^2 < 0$. Relations (1.12) show that the spectrum in each interval $S_{1,n}^k \cap S_{2,n}^k \neq \emptyset, n \geq 1$ has multiplicity 4.

(ii) In Proposition 3.3 we prove that $u_k(E_{1,p}^{0,\pm}) > 0$ and $v_k(\lambda_{1,p}^{0,\pm}) > 0$ for some $k, n$ and for some specific non-even potentials. Then relations (1.12) give $S_{1,n}^k \cap S_{2,n}^k = \emptyset$, and the last identity in (1.10) yields $E_{1,p}^{k,\pm} = \lambda_{1,p}^{0,\pm}$.

In order to describe gaps in the spectrum of $H_k$, $H$ we need

**Definition 1.** Let $g = (\lambda_1, \lambda_2)$ be a gap in the spectrum of $H_k$ or $H$.

(i) If $\lambda_1, \lambda_2$ are zeros of $D_k^+$ (or $D_k^-$), then $g$ is a periodic (or antiperiodic) gap.

(ii) If $\lambda_1, \lambda_2$ are zeros of $\rho_k$, then $g$ is a resonance gap.

(iii) If one of the numbers $\lambda_1, \lambda_2$ is a zero of $D_k^-$ and other is a zero of $D_k^+$ (or $\rho_k$), then $g$ is a $p$-mix gap (or $r$-mix gap).

In our armchair model there is no a gap $(\lambda_1, \lambda_2)$, where one of the numbers $\lambda_1, \lambda_2$ is a zero of $D_k^+$ and other is a zero of $\rho_k$.

**Theorem 1.3.** Let $k \in \mathbb{Z}_N$. Then $\sigma_{ac}(H_k) = \mathbb{R} \setminus \bigcup_{n \geq 0} G_{k,n}$, where the gaps $G_{k,n}$ satisfy:

\[
\begin{align*}
\tilde{\gamma}_0 & \subset G_{k,0} = (-\infty, E_{2,0}^{k,+}), \\
\tilde{\gamma}_n & \subset G_{k,4n} = (E_{2,2n}^{k,-}, E_{2,2n}^{k,+}), \\
G_{k,4n-3} & = (E_{2,2n-1}^{k,-}, E_{2,2n-1}^{k,+}), \\
G_{k,4n-1} & = (E_{1,2n}^{k,-}, E_{1,2n}^{k,+}) \subset \mathbb{R}, \\
G_{k,n} & = G_{N-k,n} \text{ all } k \in \mathbb{Z}_N, \\
G_{k,4n} & \subset G_{\ell,4n}, \ G_{\ell,2n-1} \subset G_{k,2n-1} \text{ all } 0 \leq k < \ell \leq \frac{N}{2}.
\end{align*}
\]

Furthermore, for some $n_0 \geq 1$ the gaps satisfy:

$G_{k,4n}$ are periodic gaps,

$G_{k,2n-1}$ are $p$-mix gaps and each $G_{k,2n-1} = \emptyset$ for $k \neq 0, n \geq n_0$

$G_{0,4n-2}$ are antiperiodic gaps and $G_{0,4n-2} = \emptyset$ for $n \geq n_0$,

$G_{k,2n-1}, k \notin \left\{0, \frac{N}{2}\right\}$ are antiperiodic, or resonance, or $r$-mix gaps, and $G_{k,4n-2}$ are resonance gaps for $n \geq n_0$,

$G_{N-4n-2}, n_0 \in \mathbb{Z}$ are antiperiodic gaps.

If $q \in L^2_{even}(0,1)$, then each $G_{k,4n-2}, k \notin \left\{0, \frac{N}{2}\right\}, n \geq 1$ is a resonance gap.

**Remark.** In Theorem 1.3 and below we let the gap $G_{k,4n-2} = \emptyset$, if $E_{1,2n-1}^{k,-} \geq E_{1,2n-1}^{k,+}$, and the similar relations for other gaps hold true.

Below we write $a_n = b_n + \ell^2(n)$ for two sequences $(a_n)_1^{\infty}, (b_n)_1^{\infty}$ iff $(a_n - b_n)_1^{\infty} \in \ell^2$. We describe the spectrum of $H$. 

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Theorem 1.4. $\sigma_{ac}(H) = \mathbb{R} \setminus \bigcup_{n \geq 0} G_n$, where the gaps $G_n = \cap_{k \in \mathbb{Z}} G_{k,n}$ and $G_n$ satisfy:

\[
G_0 = (-\infty, E_{2,0}^+) = \mathcal{G}_{0,0}, \quad G_{4n} = (E_{2,2n}^-, E_{2,2n}^+) = \mathcal{G}_{0,4n}, \quad G_{4n-2} = (E_{1,2n-1}^-, E_{1,2n-1}^+) \subset \mathcal{G}_{n}, \\
G_{4n-3} = (E_{2,2n-1}^-, E_{2,2n-1}^+) = \mathcal{G}_{m,4n-3}, \quad G_{4n-1} = (E_{1,2n}^-, E_{1,2n}^+) = \mathcal{G}_{m,4n-1},
\]

(1.15)

\[
\tilde{\gamma}_{n-1} \subset \mathcal{G}_{4n-4}, \quad \eta_n \in [E_{1,2n-1}^-, E_{1,2n-1}^+] \text{ all } n \geq 1.
\]

(1.16)

The gaps $G_{4n-2} = G_{2n-1} = \emptyset$ for all large $n \geq 1$ and the following asymptotics hold true:

\[
E_{2,2n}^\pm = E_{2,2n}^{0,\pm} = (\pi n)^2 + q_0 \pm \sqrt{\frac{2}{3} q_{sn}^2 + q_{cn}^2 + \frac{\ell^2(n)}{n}} \quad \text{as } n \to \infty,
\]

(1.17)

where $q_0 = \int_0^1 q(t)dt$, $q_{sn} = \int_0^1 q(s)\sin 2\pi nds$, $q_{cn} = \int_0^1 q(s)\cos 2\pi nds$.

There are papers about the spectral analysis of the Schrödinger operator on periodic graphs and periodic nanotubes. Molchanov and Vainberg [MV] consider Schrödinger operators with $q = 0$ on so-called necklace periodic graphs. Korotyaev and Lobanov [KL], [KL1] consider the Schrödinger operator on the zigzag nanotube. The spectrum of this operator consists of an absolutely continuous part (intervals separated by gaps) plus an infinite number of eigenvalues with infinite multiplicity. They describe all eigenfunctions with the same eigenvalue. They define a Lyapunov function, which is analytic on some Riemann surface. On each sheet, the Lyapunov function has the same properties as in the scalar case, but it has branch points (resonances). They prove that all resonances are real and they determine the asymptotics of the periodic and anti-periodic spectrum and of the resonances at high energy. They show that there exist two types of gaps: i) stable gaps, where the endpoints are periodic and anti-periodic eigenvalues, ii) unstable (resonance) gaps, where the endpoints are resonances (i.e., real branch points of the Lyapunov function). They describe all finite gap potentials. They show that the mapping: potential $\to$ all eigenvalues is a real analytic isomorphism for some class of potentials.

Moreover, Korotyaev and Lobanov [KL1] consider magnetic Schrödinger operators on zigzag nanotubes. They describe how the spectrum depends on the magnetic field. Korotyaev [K2] considers integrated density of states and effective masses for zigzag nanotubes in magnetic fields. He obtains a priori estimates of gap lengths in terms of effective masses. Kuchment and Post [KuP] consider the case of the zigzag, armchair and achiral nanotubes with even potential $q \in L^2_{even}(0,1)$. They show that the spectrum of the Schrödinger operator (on these nanotubes), as a set, coincides with the spectrum of the Hill operator.

In [BBKL] authors describe all eigenfunctions of $\mathcal{H}$ with the same eigenvalue. They define a Lyapunov function, which is analytic on some Riemann surface. On each sheet, the Lyapunov function has the same properties as in the scalar case, but it has branch points (resonances). They prove that there exist non-real and real resonances.

In the present paper we describe the absolutely continuous spectrum of $\mathcal{H}$, multiplicity of the spectrum and endpoints of the spectral bands. These results are absent in [KuP]. We show that there exist two types of gaps: i) stable gaps, where the endpoints are periodic and anti-periodic eigenvalues, ii) unstable (resonance) gaps, where the endpoints are resonances
Preliminaries

Lemma 2.1. There exists an integer \( n_0 > 1 \) such that

1. The function \( D_0^- \) given by (L.8) has exactly \( 4n_0 \) zeros, counted with multiplicities, in the domain \( \{ \lambda : |\sqrt{\lambda} - \pi n | < \pi n_0 \} \) and for each \( n > n_0 \), exactly two zeros, counted with multiplicities, in each domain \( \{ \lambda : |\sqrt{\lambda} - \pi n - \frac{\pi}{2} \pm \arcsin \frac{1}{3} | < \frac{1}{3} \} \). There are no other zeros.
2. Each function \( D_0^+ \), \( k \in \mathbb{Z}_N \) has exactly \( 4n_0 + 2 \) zeros, counted with multiplicities, in the domain \( \{ \lambda : |\sqrt{\lambda} - \pi n + \frac{\pi}{2} | < \frac{1}{3} \} \). There are no other zeros.
3. Each function \( \rho_k : k \not\in \{0, \frac{N}{2} \} \), has exactly \( 2n_0 \) zeros, counted with multiplicities, in the domain \( \{ \lambda : |\sqrt{\lambda} + \pi n | < \pi n_0 \} \), and for each \( n > n_0 \) exactly one simple zero in each domain \( \{ \lambda : |\sqrt{\lambda} - (\pi n - \frac{\pi}{2} \pm \arcsin \frac{2k}{3}) | < \frac{2k}{3} \} \). There are no other zeros.

Proof repeats the case of the zigzag nanotube [KL].

Substituting (L.7) into (L.8) we obtain for \( k \in \mathbb{Z}_N \):

\[
D_k^+ = \left( (3F - 1)^2 - 4 - F^2_\nu \right) \left( (3F + 1)^2 - 4 - F^2_\nu \right) + 16s_k^2 = (9F^2 - g_{k,1})(9F^2 - g_{k,2}),
\]

\[
D_k^- = D_0^- = \left( (3F - 1)^2 - F^2_\nu \right) \left( (3F + 1)^2 - F^2_\nu \right) = (9F^2 - h_1)(9F^2 - h_2)
\]

on \( \mathbb{R} \), where

\[
g_{k,\nu} = 5 + F^2_\nu + (-1)^\nu 2\sqrt{F^2_\nu + 4c_k^2}, \quad h_\nu = (1 + (-1)^\nu |F_-|^2).
\]

Lemma 2.2. (i) For all \( (\nu, k, n) \in \mathbb{N}_2 \times \mathbb{Z}_N \times \mathbb{N} \) the periodic and antiperiodic eigenvalues satisfy

\[
\lambda_{\nu, n-1}^{k, \pm} = \lambda_{\nu, n-1}^{N-k, \mp}, \quad \lambda_{\nu, 2n-1}^{k, \pm} = \lambda_{\nu, 2n-1}^{0, \pm}, \quad \gamma_{\nu, 2n-1}^k = \gamma_{\nu, 2n-1}^0, \quad \gamma_{1, 2n-1}^0 = \infty,
\]

\[
\lambda_{2, p+1}^{k,-} < u_k(\lambda_{2, p}^{0,-}) > 0; \quad \lambda_{2, p}^{0,+} > \lambda_{1, p+1}^{k,-} \iff u_k(\lambda_{2, p}^{0,+}) > 0.
\]

\[
\bigcup_{n \geq 1} \gamma_{\nu, n-1}^0 = \{ \lambda \in \mathbb{R} : 9F^2(\lambda) < h_\nu(\lambda) \}, \quad \bigcup_{n \geq 0} \gamma_{\nu, n+1}^k = \{ \lambda \in \mathbb{R} : 9F^2(\lambda) > g_{k,\nu}(\lambda) \}
\]
Figure 5: Functions $9F^2, g_k^\pm, h^\pm$ and $f_k$

where

$$
\gamma^k_{\nu, 0} = (\infty, \lambda_{\nu, 0}^k), \quad \gamma^k_{\nu, \pm n} = (\lambda_{\nu, n}^k, \lambda_{\nu, n}^k), \quad (\nu, n, k) \in \mathbb{N} \times \mathbb{N} \times \mathbb{Z}.
$$

(ii) If $0 \leq k < \ell \leq N$ and $n \geq 1$, then

$$
\lambda_{2n-2}^{k, +} < \lambda_{2n-2}^{\ell, +}, \quad \lambda_{1,2n-2}^{k, +} < \lambda_{1,2n-2}^{\ell, +}, \quad \lambda_{1,2n}^{k, -} < \lambda_{1,2n}^{\ell, -}, \quad \lambda_{2n}^{k, -} < \lambda_{2n}^{\ell, -}.
$$

(2.7)

**Proof.** (i) The periodic eigenvalues are zeros $D^+_k$. Using (2.1) and the identities $s_{N-k} = s_k$ we obtain the first identity in (2.3) for the periodic eigenvalues. The antiperiodic eigenvalues are zeros $D^-_k$. Using (2.1) and the definitions of $\gamma^k_{\nu, n}$, $k$ we obtain the other identities in (2.3).

Identities (2.2) give $g_{k,1} - h_1 = 2(|F_-| + 2 - \sqrt{F_0^2 + 4c_{2n}^2}) \geq 0$ on $\mathbb{R}$. Then we obtain

$$
h_1 \leq \min\{h_2, g_{k,1}\} \leq \max\{h_2, g_{k,1}\} \leq g_{k,2}.
$$

(2.8)

Identities (1.3) give $F^2 - F_0^2 = \partial_1 \varphi' = 1 + \partial_1 \varphi_1$. Then $F^2(\mu_n) = F^2(\mu_n) - 1$. The last identity and $F^2(\mu_n) \geq 1$ imply

$$
9F^2(\mu_n) - g_{k,2}(\mu_n) = 2\left(2\sqrt{F^2(\mu_n) - 1 + 4c_{k}^2} - \frac{1}{4}\right)^2 + \frac{31}{16} - 16c_{k}^2 \geq 0,
$$

which yields $g_{k,2}(\mu_n) \leq 9F^2(\mu_n)$. Estimates (2.8) and the properties of the function $F$ provide that each of the functions $9F^2 - g_{k,\nu}$, $9F^2 - h_{\nu}$, $\nu = 1, 2$ has at least one zero in each of the intervals $(-\infty, \eta_1)$, $[\eta_n, \mu_n]$, $[\mu_n, \eta_{n+1}]$, $n \geq 1$. Moreover, Lemma 2.1 shows that each
of these functions has exactly one zero in each of these intervals. Then the properties of the function $F$ and estimates (2.8) yield (2.4).

Identities (2.2) give $g_{k,1} - h_2 = 2(s_k^2 - |F_-| + \sqrt{s_k^4 + 4c_k^2} - \sqrt{F_-^2 + 4c_k^2})$. For fixed $\lambda$ we obtain $g_{k,1}(\lambda) > h_2(\lambda)$ iff $|F_-| < s_k^2$. Let $\kappa = \lambda_{0,2n-1}^0$. Estimates (2.4) show that $\kappa_n > \min\{\lambda_{0,2n-2}^k, \lambda_{2,2n-1}^0\} \leq \max\{\lambda_{2,2n-2}^k, \lambda_{2,2n-1}^0\} \leq \eta_n$. Since $(F^2)' < 0$ on $(\kappa_n, \eta_n)$, we deduce that $\kappa_n > \lambda_{2,2n-1}^0$ and $|F_-| < s_k^2$, which yields the first equivalence in (2.5). The proof of the second equivalence is similar.

Estimates (2.4), (2.8) and the properties of $F$ yield (2.6).

(ii) Identities (2.2) give $g_{k,2} < g_{\ell,2}$, $g_{\ell,1} < g_{k,1}$. The properties of $F$ yield (2.7). ■

3 Proof of Theorems 1.1-1.4

Let $R_k = \{\lambda \in \mathbb{R} : \rho_k(\lambda) > 0\}, k \neq \frac{N}{2}$. In Lemmas 3.1-3.3 we describe the set $\sigma_{k,\nu} = \{\lambda \in \mathbb{R} : F_{k,\nu}(\lambda) \in [-1,1]\}$ in terms of $F$.

**Lemma 3.1.** For all $k \in \mathbb{Z}_N$ and $\lambda \in R_k$ the following identities hold true:

$$F_{k,\nu}(\lambda) < 1 \text{ iff } 9F^2(\lambda) < g_{k,\nu}(\lambda), \quad \nu = 1, 2,$$

$$F_{k,1}(\lambda) > -1 \text{ iff } \{9F^2(\lambda) > h_1(\lambda) \text{ or } |F_-| < c_k^2\},$$

$$F_{k,2}(\lambda) > -1 \text{ iff } \left\{9F^2(\lambda) > h_2(\lambda) \text{ or } 9F^2(\lambda) < h_1(\lambda) \text{ and } |F_-| < c_k^2\right\}.$$

**Proof.** If $k = m = \frac{N}{2} \in \mathbb{Z}$, identities (1.7), (2.2) give $F_{m,\nu} - 1 = \frac{1}{2}(9F^2 - g_{m,\nu}), F_{m,\nu} + 1 = \frac{1}{2}(9F^2 - h_\nu)$, which yields (3.1)-(3.3) for $k = m$.

Let $k \neq \frac{N}{2}$. We rewrite the functions $\rho_k, F_{k,\nu} - 1$ in the form

$$\rho_k = (9F^2 - g_{k,\nu})c_k^2 + (\sqrt{F_-^2 + 4c_k^2} + (-1)^\nu c_k^2),$$

$$F_{k,\nu} - 1 = \frac{1}{2c_k^2}\left(\sqrt{\rho_k} - (-1)^\nu c_k^2 - \sqrt{F_-^2 + 4c_k^2}\right)\left(\sqrt{\rho_k} - (-1)^\nu c_k^2 + \sqrt{F_-^2 + 4c_k^2}\right).$$

These identities yields (3.1). We rewrite the functions $\rho_k, F_{k,1} + 1$ in the form

$$\rho_k = (9F^2 - h_1)c_k^2 + (|F_-| - c_k^2)^2, \quad F_{k,1} + 1 = \frac{1}{2c_k^2}\left(\sqrt{\rho_k} + c_k^2 - |F_-|\right)\left(\sqrt{\rho_k} + c_k^2 + |F_-|\right).$$

These identities imply (3.2). We rewrite the functions $\rho_k, F_{k,2} + 1$ in the form

$$\rho_k = (9F^2 - h_2)c_k^2 + (|F_-| + c_k^2)^2, \quad F_{k,2} + 1 = \frac{1}{2c_k^2}\left(\sqrt{\rho_k} - c_k^2 - |F_-|\right)\left(\sqrt{\rho_k} - c_k^2 + |F_-|\right).$$

These identities and the first identity in (3.4) give (3.3). ■

Now we describe the zeros of $\rho_k$ and the functions $F_{k,\nu}$ on the interval $\mathbb{Z}_n$. Recall the intervals $\mathbb{Z}_{k,\nu} = (\lambda_{1,2n-1}^0, r_{k,\nu})$, $\mathbb{Z}_{k,\nu}^+ = (r_{k,\nu}, \lambda_{1,2n-1}^0), n \geq 1$ (see Theorem 1.2).
Lemma 3.2. Let \( k \neq \frac{N}{2} \). Then

(i) The last identity in (1.7) gives

\[
\lambda_2 = (\lambda_{1,2n-1}^0, \lambda_{1,2n-1}^1).
\]

(ii) Identity (2.6) show that \( \rho_k \) of zeros of \( F \) imply that real zeros of \( \rho_k \) belong to the set \( \cup_{n \geq 1} \mathbb{R}_k \). Each interval \( \mathbb{R}_n, n \geq 1 \) contains even number \( \geq 0 \) of zeros of \( \rho_k \), counted with multiplicities.

(iii) If \( \rho_k(\lambda) < 0 \) for some \( \lambda \in \mathbb{R}_n, n \geq 1 \), then \( \rho_k \) has even number \( \geq 2 \) of zeros on \( \mathbb{R}_n \).

Proof. (i) The last identity in (1.7) gives

\[
\rho_k = c_k^2 (9F^2 - f_k), \quad k \neq \frac{N}{2}, \quad \text{where} \quad f_k = s_k^2 \left( 1 - \frac{F^2}{c_k^2} \right). \tag{3.10}
\]

Identities (3.10) show that zeros of \( \rho_k \) (resonances) are zeros of \( 9F^2 - f_k \). Identities (2.2), (3.10) give \( h_1 - f_k = (c_k - F_k^2)^2 \geq 0 \). Identities (2.4) and the properties of the function \( F \) imply that real zeros of \( \rho_k \) belong to the set \( \cup_{n \geq 1} \mathbb{R}_n \) and (3.5) holds. The function \( \rho_k \) has even number of zeros in \( \mathbb{R}_n \), since \( \rho_k \neq 0 \) at the points \( \lambda_{1,2n-1}^0, \lambda_{1,2n-1}^1 \).

(ii) Identity (2.6) show that \( 9F^2 < h_1 \) on \( \mathbb{R}_n \). Using the first identity in (3.4) we conclude that if \( |F_-(\lambda)| = c_k^2 \) for \( \lambda \in \mathbb{R}_n \), then \( \rho_k(\lambda) < 0 \). We obtain (3.6), since \( \rho_k > 0 \) on \( \mathbb{R}_n \).

If \( |F_-(\lambda)| > c_k^2 \) for some \( \lambda \in \mathbb{R}_n \), then (3.6) show \( |F_-(\lambda)| > c_k^2 \) for all \( \lambda \in \mathbb{R}_n \). Recall that \( 9F^2 < h_1 \) on \( \mathbb{R}_n \). Then (3.2) gives \( F_{k,1} < -1 \) on \( \mathbb{R}_n \), which yields (3.7).

If \( |F_-(\lambda)| < c_k^2 \) for some \( \lambda \in \mathbb{R}_n \), then (3.6) provide \( |F_-(\lambda)| < c_k^2 \) for all \( \lambda \in \mathbb{R}_n \). Using \( 9F^2 < h_1 \) on \( \mathbb{R}_n \) again (3.3) gives \( -1 < F_{k,2} \) on \( \mathbb{R}_n \). We obtain (3.8).

Suppose that \( \mathbb{R}_n \in R_k \), i.e. \( \rho_k > 0 \) on \( \mathbb{R}_n \). Estimates (2.4) yield \( \eta_n \in \mathbb{R}_n \), hence \( \rho_k(\eta_n) > 0 \). Note that \( \rho_0(\eta_n) = 0 \), hence the condition \( \mathbb{R}_n \in R_0 \) is not fulfilled for all \( n \). In this reason we assume below \( k \neq 0 \).

The last identity in (1.7) gives \( F_2^2(\eta_n) = s_k^{-2} \rho_k(\eta_n) + c_k^2 > c_k^2 \), which yield \( |F_-(\eta_n)| > c_k^2 \). Using \( 9F^2 < h_1 \) on \( \mathbb{R}_n \) and the first identity in (3.4) again we conclude that if \( |F_-(\lambda)| = c_k^2 \) for \( \lambda \in \mathbb{R}_n \), then \( \rho_k(\lambda) < 0 \), which yields \( \text{sign}(|F_+| - c_k^2) = \text{const on } \mathbb{R}_n \). Thus \( |F_-(\lambda)| < c_k^2 \) for all \( \lambda \in \mathbb{R}_n \) and we have the first estimate in (3.9). Relation (3.2) gives \( F_{k,1} < -1 \) on \( \mathbb{R}_n \), which yields the second estimate in (3.9).

(iii) Using relation (3.9) we deduce that if \( \rho_k(\lambda) < 0 \) for some \( \lambda \in \mathbb{R}_n = [\lambda_{1,2n-1}^0, \lambda_{1,2n-1}^1] \), then \( \mathbb{R}_n \not\subset R_k \). Hence there exists \( \lambda \in \mathbb{R}_n \) such that \( \rho_k(\lambda) < 0 \). On the other hand \( \rho_k(\lambda_{1,2n-1}^0) \geq 0 \), which yields the needed statement. \( \blacksquare \)
For each \((k, \nu) \in \mathbb{Z}_N \times \mathbb{N}_2\) we introduce the sets

\[
\mathcal{S}_{k,\nu} = \bigcup_{n \geq 1} \left[ \lambda_{k,2n-1}^{\nu,0}, \lambda_{k,2n-1}^{\nu,-1} \right] \cup \left[ \lambda_{k,2n-1}^{\nu,0}, \lambda_{k,2n}^{\nu,-1} \right], \quad \mathcal{S}_{k}^R = \bigcup_{\sigma = \pm, n \in \mathbb{N}_2^\nu} \mathcal{S}_{k,n}^\sigma,
\]

where \(N^\pm_k = \{n \in \mathbb{N} : v_k(\lambda_{1,2n-1}^{\nu,0}) < 0\}\). The set \(\mathcal{S}_{k,\nu}\) is a part of \(\sigma_{k,\nu}\), where the periodic and antiperiodic eigenvalues are endpoints of bands. The set \(\mathcal{S}_{k}^R\) is an “unstable” part of \(\sigma_{k,\nu}\).

**Lemma 3.3.** For each \((\nu, k) \in \mathbb{N}_2 \times \mathbb{Z}_N\) the following identities hold true:

\[
\mathcal{S}_{k,\nu} = \{ \lambda \in \mathbb{R} : h_\nu(\lambda) \leq 9F^2(\lambda) \leq g_{k,\nu}(\lambda) \},
\]

\[
\mathcal{S}_k^R = \{ \lambda \in R_k : 9F^2(\lambda) \leq h_1(\lambda) \text{ and } v_k(\lambda) \leq 0 \}, \quad k \neq \frac{N}{2}, \quad \text{and} \quad \mathcal{S}_{k,\nu}^R = \emptyset.
\]

**Proof.** Identities (2.6) give (3.12). If \(m = \frac{N}{2} \in \mathbb{Z}\), then \(c_m = 0, \ v_m(\lambda) = |F_-(\lambda)| \geq 0\) and \(N^\pm_k = \emptyset\), which yields \(\mathcal{S}_k^R = \emptyset\). The first identity in (2.6) gives \(\bigcup_{n \geq 1} \mathcal{S}_n = \{ \lambda \in \mathbb{R} : 9F^2(\lambda) < h_1(\lambda) \}\). Then (3.7)-(3.9) provide (3.13) for \(k \neq \frac{N}{2}\). Identities (3.1)-(3.3) yield (3.14). We prove our main results.

**Proof of Theorem 1.1.** Identities (3.11)-(3.14) give

\[
\sigma_{k,1} = \bigcup_{n \geq 1} (S_{1,2n-1}^k \cup S_{1,2n}^k), \quad \sigma_{k,2} = (\bigcup_{\sigma = \pm, n \in \mathbb{N}_2^\nu} \mathcal{S}_{k,n}^{\sigma}) \cup (\bigcup_{n \geq 1} (S_{2,2n-1}^k \cup S_{2,2n}^k)),
\]

where \(S_{1,2n-1}^k = [\lambda_{k,2n-1}^{\nu,0}, \lambda_{k,2n-1}^{\nu,-1}] \cup \mathcal{S}_{k,n}^{\nu,-1}\) and \(S_{1,2n}^k = [\lambda_{k,2n}^{\nu,0}, \lambda_{k,2n}^{\nu,-1}] \cup \mathcal{S}_{k,n}^{\nu,0}\). Then (1.10) holds true. Using (1.6) and \(\mathcal{S}_{k,n}^{\nu,-1} \subset S_{k,1,2n-1}^k, \mathcal{S}_{k,n}^{\nu,0} \subset S_{k,1,2n-1}^k\), we obtain \(\sigma_{ac}(H_k) = \sigma_{k,1} \cup \sigma_{k,2} = \bigcup_{\nu \in \mathbb{N}_2} (\bigcup_{n \geq 1} S_{k,\nu}^{\nu})\). Estimates (2.4) give (1.11). Relations (2.5) provide (1.12). We prove Theorem 1.2. The last identity in (1.10) together with (3.8) imply \(E_{1,p}^{k,\pm} = r_{k,n}^{\pm}\) iff \(-1 < F_{k,2} < F_{k,1}\) on \(\mathcal{S}_{k,n}^{\nu}\). Identity (3.11) shows that \(\mathcal{S}_{k,n}^{\nu} \subset \mathcal{S}_k^R\). Identity (3.13) yields \(9F^2 \leq h_1\) on \(\mathcal{S}_{k,n}^{\nu}\). Relations (3.2) give \(F_{k,2} < F_{k,1} < 1\) on \(\mathcal{S}_{k,n}^{\nu}\). Then the spectrum in \(\mathcal{S}_{k,n}^{\nu}\) has multiplicity 4. Suppose that \(E_{1,p}^{k,\pm} \neq r_{k,n}^{\pm}\). Then the last identity in (1.11) show \(v_k(\lambda_{1,2n-1}^{\nu,0}) \geq 0\). Relation (3.7) yields \(F_{k,2} < F_{k,1} < 1\) on \(\mathcal{S}_{k,n}^{\nu}\). Hence the interval \(\mathcal{S}_{k,n}^{\nu}\) lies in a gap of \(H_k\).

Using (1.10) we rewrite \(\mathcal{S}_{k,\nu}\) (see (3.11)) in the form \(\mathcal{S}_{k,\nu} = \bigcup_{n \geq 1} (E_{\nu,2n-2}^{k,-} \cup E_{\nu,2n-1}^{k,0} \cup E_{\nu,2n}^{k,-} \cup E_{\nu,2n+1}^{k,0})\). Estimates (1.11) show that

\[
\mathcal{S}_{k} = \mathcal{S}_{k,1} \cup \mathcal{S}_{k,2} = \left( \bigcup_{n : E_{2p}^{k,0} < E_{1,p-1}^{k,0}} (E_{2p}^{k,0} \cup E_{1,p-1}^{k,0}) \right) \cup \left( \bigcup_{n : E_{2p}^{k,0} < E_{1,p+1}^{k,0}} (E_{2p}^{k,0} \cup E_{1,p+1}^{k,0}) \right).
\]

Identity (3.14) give \(F_{k,\nu} \in [-1, 1]\) on \(\mathcal{S}_{k,\nu}\). Then \(F_{k,\nu} \in [-1, 1]\) for \(\nu = 1, 2\) on \(\mathcal{S}_{k}\). Hence the spectrum on this set has multiplicity 4. The spectrum on \((\mathcal{S}_{k,1} \cup \mathcal{S}_{k,2}) \setminus \mathcal{S}_{k}\) has multiplicity 2. ■
We need the following well known asymptotics (see, for example, [K])

\[ F(\lambda) = \cos \sqrt{\lambda} + \frac{q_0 \sin \sqrt{\lambda}}{2\sqrt{\lambda}} + O(e^{1\text{Im}\sqrt{\lambda}}), \]

\[ F_-(\lambda) = -\frac{1}{2\sqrt{\lambda}} \int_0^1 \sin \sqrt{\lambda}(1-2t)q(t)dt + O(e^{1\text{Im}\sqrt{\lambda}}), \quad |\lambda| \to \infty. \] (3.15)

**Proof of Theorem 1.3.** Estimates (2.4) show that the intervals \( G^k_{\nu,n} = (E^k_{\nu,n}^-, E^k_{\nu,n}^+) \), \((\nu, n) \in \mathbb{N}_2 \times \mathbb{N},\) satisfy:

\[ G^k_{1,0} \cap G^k_{2,0} = \emptyset \quad \text{for} \quad m \not\in \{0, 1\}, \quad G^k_{1,2n-1} \cap G^k_{2,2n} = \emptyset \quad \text{for} \quad m \not= 2n - 1, \]

\[ G^k_{1,2n} \cap G^k_{2,m} = \emptyset \quad \text{for} \quad m \not\in \{2n - 1, 2n, 2n + 1\}. \]

Then the gaps \( G_{k,n}, n \geq 0 \) in the spectrum \( H_k \) are given by

\[ G_{k,0} = G^k_{1,0} \cap G^k_{2,0}, \quad G_{k,2n} = G^k_{1,n} \cap G^k_{2,2n}, \quad G_{k,4n-3} = G^k_{1,2n-2} \cap G^k_{2,2n-1}, \quad G_{k,4n-1} = G^k_{1,2n} \cap G^k_{2,2n-1}, \]

\( n \geq 1, \) which yields all identities in (1.13). Estimates (2.3) give all inclusions in (1.13). Lemma 2.2 and relations (3.5), (2.7) give (1.14). Identities (1.10) show that \( G_{k,4n} \) are periodic gaps, \( G_{k,2n-1} \) are p-mix gaps and \( G_{k,4n-2} \) are antiperiodic, or resonance, or r-mix gaps. Asymptotics (3.13) and estimates (1.12) give that \( E^c_{k,4n-3} > E^+_k,4n-3 \) and \( E^-_{k,4n-1} > E^+_k,4n-1 \) for \( k \neq 0 \) and large \( n > 1. \) Hence \( G_{k,2n-1} = \emptyset \) for such \( k, n. \)

Recall that \( r_{0,n}^- = r_{0,0}^+ = \eta_n. \) Identities (1.10) give \( E^0_{1,p} = \begin{cases} \lambda_{1,p}^0 \quad \text{if} \quad v_0(\lambda_{1,p}^0) > 0 \\ \eta_n \quad \text{if} \quad v_0(\lambda_{1,p}^0) < 0 \end{cases}. \)

Hence \( G_{0,4n-2} \) are antiperiodic gaps or \( G_{0,4n-2} = \emptyset. \) Moreover, \( E^0_{1,p} = E^0_{1,0} = \eta_n \) for all large \( n \geq 1. \) Hence \( G_{0,4n-2} = \emptyset \) for large \( n \geq 1. \)

Since \( c_m = 0, m = \frac{N}{2} \in \mathbb{Z}, \) identities (1.10) provide \( E^{m,\pm}_{1,p} = \lambda^{m,\pm}_{1,p}. \) Hence \( G_{m,4n-2} \) are antiperiodic gaps.

For \( k \neq \{0, \frac{N}{2}\} \) identities (1.10) give \( G_{k,4n-2} \) are antiperiodic, or resonance, or r-mix gaps, and asymptotics (3.15) show that \( G_{k,4n-2} \) are resonance gaps.

If \( q \in L^2_{\text{even}}(0,1), \) then \( F_- = 0 \) and \( v_k < 0, k \neq \frac{N}{2}. \) Identities (1.10) show that \( E^k_{1,p} = r_{k,n}^\pm \) in this case. The last identity in (1.7) yield \( \rho_k = (9F^2 - s_k^2)c_k^2. \) Properties on the function \( F \) show that \( r_{-n,k}^- < r_{k,n}^+ \) for \( k \neq 0, \frac{N}{2} \) and all \( n \geq 1. \) Then \( G_{k,4n-2} = (r_{-n,k}^-, r_{k,n}^+), n \geq 1 \) are resonance gaps. \( \square \)

**Proof of Theorem 1.4.** Recall that the operator \( H \) is unitarily equivalent to \( H = \bigoplus_1^NH_k. \) Relations (1.14) provide \( \sigma_{ac}(H) = \mathbb{R} \setminus \cup_{n \geq 0}G_{n,} \) gap \( G_n = \cap_{k \in \mathbb{Z}_N} G_{k,n}. \) The second relations in (1.14) show \( G_{4n} = G_{0,4n}, n \geq 0. \) The third relations in (1.14) imply \( G_{2n-1} = G_{m,2n-1}, n \geq 1. \) the relations \( \hat{G}_{k,n} \subset \hat{\mathcal{N}}_n \) give \( G_{2n-1} \subset \hat{\mathcal{N}}. \) Thus, we have proved all relations in (1.15).

The relations \( \hat{\mathcal{N}}_n \subset G_{k,4n}, \eta_n \in [E^k_{1,2n-1}, E^k_{1,2n-1}] \) give the corresponding relations \( \gamma_n \subset G_{4n}, \eta_n \in [E^1_{1,2n-1}, E^1_{1,2n-1}], \) which yields (1.10). By Theorem 1.3 \( G_{m,2n-1} = G_{0,4n-2} = \emptyset \) for large \( n \geq 1, \) which implies \( G_{4n-2} = G_{2n-1} = \emptyset \) for large \( n \geq 1. \)
In order to prove asymptotics (1.17) we assume that \( \int_0^1 q(t)dt = 0 \). Identities (2.1) and Lemma 2.1(ii) show that \( \lambda_{2,2n}^{0,\pm} \) are zeros of the equation

\[
3F(\lambda) = (-1)^n(1 + \sqrt{F^2(\lambda) + 4}),
\]

and \( \lambda_{2,2n}^{0,\pm} = (\pi n + \varepsilon_{n}^{\pm})^2 \), where \( |\varepsilon_{n}^{\pm}| \leq \frac{1}{3} \) for large \( n \). Let \( \lambda = \lambda_{2,2n}^{0,\pm} \) and \( \varepsilon = \varepsilon_{n}^{\pm} \). Asymptotics (3.15) give

\[
F(\lambda) = (-1)^n + O(\varepsilon^2) + O(n^{-2}), \quad F_{-}(\lambda) = O(n^{-1}).
\]

Substituting these asymptotics into (3.16) we get \( \varepsilon = O(n^{-1}) \). Using the standard calculations (see [K]) we obtain

\[
F(\lambda) = (-1)^n \left( 1 + \frac{q_{2n}^2 + q_{cn}^2}{2(2\pi n)^2} - \frac{\varepsilon^2}{2} \right) + \frac{\ell^2(n)}{n^3}, \quad F_{-}(\lambda) = \frac{(-1)^n q_{sn}}{2\pi n} + \frac{\ell^2(n)}{n^2}.
\]

Substituting the last asymptotics into (3.16) we obtain \( \varepsilon^2 = \frac{2q_{2n}^2 + q_{cn}^2}{2(2\pi n)^2} + \frac{\ell^2(n)}{n^3} \), which yields \( \lambda_{2,2n}^{0,\pm} = (\pi n)^2 \pm \sqrt{\frac{2q_{2n}^2 + q_{cn}^2}{2(2\pi n)^2} + \frac{\ell^2(n)}{n^3}} \). Identity (1.15) yield \( \lambda_{2,2n}^{0,\pm} = E_{2,2n}^{0,\pm} \). Asymptotics (1.17) follow.

Now we prove Remark to Theorem 1.1 1.2

**Lemma 3.4.** Let \( k \neq \frac{N}{2} \). Then for each \( n : \kappa_n \not\in R_k \) the following relations hold true:

\[
v_k(\lambda_{1,2n-1}^{0,\pm}) \geq 0 \iff F_{k,1}(r_{k,n}^{\pm}) = F_{k,2}(r_{k,n}^{\pm}) \leq -1, \quad (3.17)
\]

\[
v_k(\lambda_{1,2n-1}^{0,\pm}) < 0 \iff F_{k,1}(r_{k,n}^{\pm}) = F_{k,2}(r_{k,n}^{\pm}) \in (-1, -\frac{1}{2}], \quad (3.18)
\]

Moreover, if \( q \) is even, i.e. \( q(1-t) = q(t) \), then \( F_{k,1}(r_{k,n}^{\pm}) = F_{k,2}(r_{k,n}^{\pm}) \in (-1, -\frac{1}{2}] \).

**Proof.** Let \( r = r_{k,n}^{\pm} \). Recall \( \rho_k(r) = 0 \). Identities (1.7) yield \( (9F^2(r) - s_k^2)c_k^2 = -s_k^2F^2(r) \leq 0 \), then \( 9F^2(r) \leq s_k^2 \). Moreover,

\[
F_{k,1}(r) = F_{k,2}(r) = \xi_k(r) = \frac{9F^2(r) - F^2(r) - 1}{2} - s_k^2 \leq -\frac{1}{2}.
\]

Relations (3.7), (3.8) give that if \( v_k(\lambda_{1,p}^{0,\pm}) > 0 \), then \( F_{k,\nu}(r) < -1 \), and if \( v_k(\lambda_{1,p}^{0,\pm}) < 0 \), then \( F_{k,\nu}(r) > -1, \nu = 1, 2 \).

Conversely, let \( F_{k,\nu}(r) < -1 \). Then (3.2) yield \( v_k(r) > 0 \). Identities (3.6) give \( v_k(r) > 0 \) on \( \kappa_{k,n}^{\pm} \), then \( v_k(\lambda_{1,p}^{0,\pm}) \geq 0 \). Let \( F_{k,\nu}(r) > -1 \). Identity (2.6) show that \( 9F^2(r) < h_1(r) \). Then (3.2) yield \( v_k(r) < 0 \). Identities (3.6) give \( v_k(r) < 0 \) on \( \kappa_{k,n}^{\pm} \), then \( v_k(\lambda_{1,p}^{0,\pm}) < 0 \). Relations (3.17), (3.18) are proved.

If \( q \in L^2_{even}(0,1) \), then \( F_- = 0 \) (see [MW]) and \( v_k < 0, k \neq \frac{N}{2} \). Then (3.18) gives \( F_{k,1}(r) = F_{k,2}(r) = -\frac{s_k^2 + 1}{2} \in (-1, -\frac{1}{2}] \).
Proposition 3.5. Let \( k \not\in \{0, \frac{N}{2}\}, q = q_e = \frac{1}{\varepsilon} \delta(t - \frac{1}{2} - c_k \varepsilon - \varepsilon^2), \varepsilon \neq 0 \) and let \( n_0 > 1 \). Then there exists \( \varepsilon_1 > 0 \) such that for all \( \varepsilon \in (-\varepsilon_1, \varepsilon_1) \setminus \{0\}, 1 \leq n \leq n_0 \) the following relations hold true:

\[
v_k(\lambda^{0,\pm}_{1,2n-1}, q_e) > 0, \quad E^{k,\pm}_{1,2n-1}(q_e) = \lambda^{0,\pm}_{1,2n-1}(q_e),
\]

(3.19)

\[
u_\ell(E^{0,\pm}_{2,2n-1}, q_e) > 0, \quad S^{\ell}_{1,n}(q_e) \cap S^{\ell}_{2,n}(q_e) \neq \emptyset, \quad \text{all } 0 \leq \ell < \frac{N}{2} - k.
\]

(3.20)

**Proof.** If \( q_e = \frac{1}{\varepsilon} \delta(t - a), v \neq 0, a \in (0, 1) \), then we have (see, for example [BBKL])

\[
F_-(\lambda, q_e) = \frac{2z_k \varepsilon}{(2z_k \varepsilon)^{2z_k}} = c_k + \varepsilon + O(\varepsilon^2) \text{ as } |\varepsilon| \to 0,
\]

(3.21)

uniformly on \( |z| \leq \pi n_0 \). Using this asymptotics we deduce that there exists \( \varepsilon_1 > 0 \) such that if \( |\varepsilon| < \varepsilon_1 \), then \( |F_-(\lambda)| > c^2_k \) and \( v_k(\lambda) > 0 \) for all \( 0 \leq \lambda < (\pi n_0)^2 \). Using (1.10) we obtain (3.19). Moreover, \( |F_-(\lambda)| > s_\ell^2 \) for all \( \ell < \frac{N}{2} - k \) and \( 0 \leq \lambda < (\pi n_0)^2 \). Thus, we obtain \( u_\ell(\lambda) > 0 \) for such \( \ell, \lambda \). Then (1.12) gives (3.20). \( \blacksquare \)

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