SPECTRAL BAND LOCALIZATION FOR SCHRÖDINGER OPERATORS ON DISCRETE PERIODIC GRAPHS

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Abstract. We consider Schrödinger operators on periodic discrete graphs. It is known that the spectrum of these operators has band structure. We describe a localization of spectral bands and estimate the Lebesgue measure of the spectrum in terms of eigenvalues of Dirichlet and Neumann operators on a fundamental domain of the periodic graph. The proof is based on the Floquet decomposition of Schrödinger operators and the minimax principle.

1. Introduction and main results

We consider Schrödinger operators with periodic potentials on $\mathbb{Z}^d$-periodic discrete graphs, $d \geq 2$. Such operators are of interest due to their applications to problems of physics and chemistry. It is known that the spectrum of Schrödinger operators consists of an absolutely continuous part and a finite number of flat bands (i.e., eigenvalues of infinite multiplicity). The absolutely continuous spectrum consists of a finite number of intervals (spectral bands) separated by gaps. Here we have a well-known problem: to estimate the spectral bands and gaps in terms of graph parameters and potentials. In the case of the Schrödinger operators $-\Delta + Q$ with a periodic potential $Q$ on $\mathbb{R}^d$ there are two-sided estimates of potentials in terms of gap lengths only at $d = 1$ in [K98], [K03]. We do not know other estimates.

In order to describe Dirichlet-Neumann bracketing in the simplest case we consider the Schrödinger operators $T = -d^2/dx^2 + q(x)$, acting on $L^2(\mathbb{R})$, where $q \in L^2(0, 1)$ is the 1-periodic real potential. The following well-known material can be found in many books; see, e.g., Levitan-Sargsyan [LS75]. The spectrum of $T$ is absolutely continuous and consists of intervals $\sigma_n = [a_n^-, a_n^+]$, where

$$a_n^+ - 1 < a_n^- \leq a_n^+, \quad n \geq 1, \quad a_n^\pm = (\pi n)^2 + O(1) \quad \text{as } n \to \infty.$$  

Consider the Sturm-Liouville problem on the unit interval with the Dirichlet boundary conditions:

$$-f'' + qf = \lambda f, \quad f(0) = f(1) = 0, \quad \lambda \in \mathbb{C},$$

where $q$ is the periodic potential restricted on the unit interval. Let $D_n, n \geq 1$, be the Dirichlet eigenvalues, that is, the eigenvalues of the problem (1.2).
We also consider the Sturm-Liouville problem on the unit interval with the Neumann boundary conditions:

\begin{equation}
- f'' + qf = \lambda f, \quad f'(0) = f'(1) = 0, \quad \lambda \in \mathbb{C}.
\end{equation}

Let $N_n, n \geq 1$, be the Neumann eigenvalues, that is, the eigenvalues of the problem \eqref{1.3}. It is well known that the Dirichlet and Neumann eigenvalues satisfy: $N_n < D_n$, and $N_{n+1}, D_n \in [a_n^-, a_n^+]$ for all $n \geq 1$. Thus we obtain

\begin{equation}
\sigma_n \subset [N_n, D_n], \quad \forall \ n \in \mathbb{N}.
\end{equation}

This is a simple example of Dirichlet-Neumann bracketing. For more complicated examples see \cite{P03, S78} and the references therein.

For the case of periodic graphs we know only two papers about estimates of spectrum and gaps:

1) Lledó and Post \cite{LP08} obtained Dirichlet-Neumann bracketing for the Laplacian on periodic metric graphs. Via an explicit Cattaneo correspondence \cite{C97} they determined Dirichlet-Neumann bracketing for the normalized Laplacian on periodic discrete graphs. Finally, they wrote “It is a priori not clear how the eigenvalue bracketing can be seen directly for discrete Laplacians, so our analysis may serve as an example of how to use metric graphs to obtain results for discrete graphs” (p. 809 in \cite{LP08}).

2) Korotyaev and Saburova \cite{KS13} considered Schrödinger operators on the discrete graphs and estimated the Lebesgue measure of their spectrum in terms of geometric parameters of the graph only.

In our paper we do not use the Cattaneo correspondence. We construct Dirichlet-Neumann bracketing and estimate directly spectral band positions and the Lebesgue measure of the spectrum of discrete Schrödinger operators in terms of the spectrum of Dirichlet and Neumann operators on a fundamental domain of the periodic graph. These estimates in some cases allow us to determine the existence of gaps in the spectrum of Schrödinger operators. Note that even for Laplacians it is new and the Lledó-Post result \cite{LP08} does not work here, since our Laplacian is not normalized and then there is no Cattaneo correspondence between the spectra of Laplacians on discrete and metric graphs.

1.1. Schrödinger operators on periodic graphs. Let $\Gamma = (V, E)$ be a connected graph, possibly having loops and multiple edges, where $V$ is the set of its vertices and $E$ is the set of its unoriented edges. An edge connecting vertices $u$ and $v$ from $V$ will be denoted as the unordered pair $(u, v) \in E$ and is said to be incident to the vertices. Vertices $u, v \in V$ will be called adjacent and denoted by $u \sim v$, if $(u, v) \in E$. For each vertex $v \in V$ we define the degree $\kappa_v = \deg v$ as the number of all its incident edges from $E$ (here a loop is counted twice). Below we consider locally finite $\mathbb{Z}^d$-periodic graphs $\Gamma$, i.e., graphs satisfying the following conditions:

1) the number of vertices from $V$ in any bounded domain $\subset \mathbb{R}^d$ is finite;
2) the degree of each vertex is finite;
3) there exists a basis $a_1, \ldots, a_d$ in $\mathbb{R}^d$ (the so-called periods of $\Gamma$) such that $\Gamma$ is invariant under translations through the vectors $a_1, \ldots, a_d$:

$$
\Gamma + a_s = \Gamma, \quad \forall \ s \in \mathbb{N}_d = \{1, \ldots, d\}.
$$
From this definition it follows that a \( \mathbb{Z}^d \)-periodic graph \( \Gamma \) is invariant under translations through any integer vector (in the basis \( a_1, \ldots, a_d \)):

\[ \Gamma + m = \Gamma, \quad \forall m \in \mathbb{Z}^d. \]

Let \( \ell^2(V) \) be the Hilbert space of all functions \( f : V \to \mathbb{C} \), equipped with the norm

\[ \|f\|_{\ell^2(V)}^2 = \sum_{v \in V} |f(v)|^2 < \infty. \]

We define the self-adjoint Laplacian (or the Laplace operator) \( \Delta \) on \( \ell^2(V) \) by

\[ (\Delta f)(v) = \sum_{(v, u), e \in E} (f(v) - f(u)) \quad \forall v \in V. \]  

We recall the basic facts (see [Me94], [M92], [MW89]) for both finite and periodic graphs: the point \( \theta \) belongs to the spectrum \( \sigma(\Delta) \) and \( \sigma(\Delta) \) is contained in \([0, 2\kappa_+]\), i.e.,

\[ 0 \in \sigma(\Delta) \subset [0, 2\kappa_+], \quad \kappa_+ = \sup_{v \in V} \deg v < \infty. \]

We consider the Schrödinger operator \( H \) acting on the Hilbert space \( \ell^2(V) \) and given by

\[ H = \Delta + Q, \]  

\[ (Qf)(v) = Q(v)f(v) \quad \forall v \in V, \]

where we assume that the potential \( Q \) is real valued and satisfies

\[ Q(v + a_s) = Q(v), \quad \forall (v, s) \in V \times \mathbb{N}_d. \]  

1.2. **Spectrum of Schrödinger operators.** We define the fundamental graph \( \Gamma_F = (V_F, \mathcal{E}_F) \) of the periodic graph \( \Gamma \) as a graph on the surface \( \mathbb{R}^d/\mathbb{Z}^d \) by

\[ \Gamma_F = \Gamma/\mathbb{Z}^d \subset \mathbb{R}^d/\mathbb{Z}^d. \]

The fundamental graph \( \Gamma_F \) has the vertex set \( V_F \) and the set \( \mathcal{E}_F \) of unoriented edges, which are finite. In the space \( \mathbb{R}^d \) we consider a coordinate system with the origin at some point \( O \). The coordinate axes of this system are directed along the vectors \( a_1, \ldots, a_d \). Below the coordinates of all vertices of \( \Gamma \) will be expressed in this coordinate system. We identify the vertices of the fundamental graph \( \Gamma_F = (V_F, \mathcal{E}_F) \) with the vertices of the graph \( \Gamma = (V, \mathcal{E}) \) from the set \([0, 1)^d \) by

\[ V_F = [0, 1)^d \cap V = \{v_1, \ldots, v_\nu\}, \quad \nu = \#V_F < \infty, \]

where \( \#A \) is the number of elements of the set \( A \).

The Schrödinger operator \( H = \Delta + Q \) on \( \ell^2(V) \) has the decomposition into a constant fiber direct integral

\[ \ell^2(V) = \frac{1}{(2\pi)^d} \int_{\mathbb{T}^d} \ell^2(V_F) \, d\vartheta, \quad \mathcal{U} H U^{-1} = \frac{1}{(2\pi)^d} \int_{\mathbb{T}^d} \Delta(d\vartheta) d\vartheta, \]

\[ \mathbb{T}^d = \mathbb{R}^d/(2\pi \mathbb{Z})^d, \]

for some unitary operator \( U \). Here \( \ell^2(V_F) = \mathbb{C}^\nu \) is the fiber space and the Floquet \( \nu \times \nu \) matrix \( H(\vartheta) \) (i.e., a fiber matrix) is given by

\[ H(\vartheta) = \Delta(\vartheta) + q, \quad q = \text{diag}(q_1, \ldots, q_\nu), \quad \forall \vartheta \in \mathbb{T}^d, \]

and \( q_j \) denote the values of the potential \( Q \) on the vertex set \( V_F \) by

\[ Q(v_j) = q_j, \quad j \in \mathbb{N}_\nu = \{1, \ldots, \nu\}. \]
The decomposition (1.11) is standard and follows from the Floquet-Bloch theory [RS78]. The precise expression of the Floquet matrix $\Delta(\vartheta)$ for the Laplacian $\Delta$ is given by (2.5). Each Floquet $\nu \times \nu$ matrix $H(\vartheta)$, $\vartheta \in \mathbb{T}^d$, has $\nu$ eigenvalues labeled by

$$\lambda_1(\vartheta) \leq \ldots \leq \lambda_\nu(\vartheta).$$

Note that the spectrum of the Floquet matrix $H(\vartheta)$ does not depend on the choice of the coordinate origin $O$. Each $\lambda_n(\cdot)$, $n \in \mathbb{N}_\nu$, is a real and continuous function on the torus $\mathbb{T}^d$ and creates the spectral band $\sigma_n(H)$ given by

$$\sigma_n(H) = [\lambda_n^-, \lambda_n^+] = \lambda_n(\mathbb{T}^d).$$

Thus, the spectrum of the operator $H$ on the periodic graph $\Gamma$ is given by

$$\sigma(H) = \bigcup_{\vartheta \in \mathbb{T}^d} \sigma(H(\vartheta)) = \bigcup_{n=1}^\nu \sigma_n(H).$$

Note that if $\lambda_n(\cdot) = C_n = \text{const}$ on some set $\mathcal{B} \subset \mathbb{T}^d$ of positive Lebesgue measure, then the operator $H$ on $\Gamma$ has the eigenvalue $C_n$ with infinite multiplicity. We call $C_n$ a flat band. Thus, the spectrum of the Schrödinger operator $H$ on the periodic graph $\Gamma$ has the form

$$\sigma(H) = \sigma_{ac}(H) \cup \sigma_{fb}(H),$$

where $\sigma_{ac}(H)$ is the absolutely continuous spectrum, which is a union of non-degenerate intervals, and $\sigma_{fb}(H)$ is the set of all flat bands (eigenvalues of infinite multiplicity). An open interval between two neighboring non-degenerate spectral bands is called a spectral gap.

1.3. Localization of spectral bands for Schrödinger operators. A subgraph $\Gamma_1 = (V_1, \mathcal{E}_1)$ of $\Gamma$ is called a fundamental domain of $\Gamma$ if it satisfies the following conditions:

1) $\Gamma_1 = (V_1, \mathcal{E}_1)$ is a finite connected graph with an edge set $\mathcal{E}_1$ and a vertex set $V_1 \supset V_F$;

2) $\Gamma_1$ does not contain any $\mathbb{Z}^d$-equivalent edges;

3) $\bigcup_{m \in \mathbb{Z}^d} (\Gamma_1 + m) = \Gamma$.

Remark. It is possible to omit the “convenient” condition $V_F \subset V_1$ in the definition of the fundamental domain and to consider a wider class of the fundamental domains. In this case the main results still hold true, but the proof of the main results will be a bit more complicated.

The fundamental domain $\Gamma_1$ is not uniquely defined and we fix one of them. Let $x_v^1$ be the degree of the vertex $v \in V_1$ on $\Gamma_1$. A vertex $v \in V_1$ is called an inner vertex of $\Gamma_1$, if $x_v = x_v^1$, i.e., if all its incident edges $e \in \mathcal{E}$ also belong to $\mathcal{E}_1$. Denote by $V_o$ the set of all inner vertices of $\Gamma_1$. We define a boundary $\partial V_1$ of $\Gamma_1$ by the standard identity:

$$\partial V_1 = V_1 \setminus V_o.$$

Example 1. We consider the square lattice $\Gamma$. We choose the periods of the graph $a_1, a_2$ as shown in Figure [1]. A fundamental domain $\Gamma_1$, the inner vertices and the boundary are shown in Figure [1]. In this simple situation the definitions of $V_o$ and $\partial V_1$ are quite clear and natural. But for more complicated graphs the situation may be rather difficult (see Figure [3]).
Figure 1. The square lattice $\Gamma$ and its fundamental domain $\Gamma_1$; the vertices of the graph $\Gamma_1$ are big points (black and white); the edges of $\Gamma_1$ are marked by bold lines. The inner vertices are black points, the boundary vertices are white points.

Figure 2. a) The fundamental domain $\Gamma_1$ of the hexagonal lattice; $V_1 = \{v_1, v_2, v_3, v_4\}$, the inner vertex set and the boundary are $V_o = \{v_1\}$, $\partial V_1 = \{v_2, v_3, v_4\}$, respectively. b) Another finite graph $\Gamma_1$ of the hexagonal lattice; $V_o = \emptyset$, $\partial V_1 = V_1 = \{v_1, v_2, v_3, v_4\}$. c) The fundamental graph $\Gamma_F$ of the hexagonal lattice; the vertices of $\Gamma_F$ are black.

Example 2. For the hexagonal lattice with periods $a_1, a_2$ (see Figure 2) we can choose a fundamental domain $\Gamma_1$ by two different not isomorphic ways (see Figure 2a, b). The numbers of the inner vertices and the boundary vertices depend on the choice of the graph $\Gamma_1$. The first graph $\Gamma_1$ (see Figure 2a) has one inner vertex and 3 boundary vertices. But for another graph $\Gamma_1$ (see Figure 2b) the set of the inner vertices is empty and $V_1 = \partial V_1$.

Remark. 1) If the graph $\Gamma_1$ is “rather big”, then the number of the inner vertices is significantly greater than the number of the boundary vertices. If the graph $\Gamma_1$
is “rather small”, then the set $V_o$ may be empty and all vertices of $\Gamma_1$ are the boundary vertices (see Theorem 1.2 ii). But the boundary never disappears. 

2) $V_o \subset V_F$ (for more details see Lemma 2.4).

On the finite graph $\Gamma_1$ we define two self-adjoint operators $H_1$ and $H_\phi$:

1) The Neumann operator $H_1$ on $\ell^2(V_1)$ is defined by

$$(1.18) \quad H_1 = \Delta_1 + Q, \quad \Delta_1 = \sqrt{\rho} \Delta_s \sqrt{\rho},$$

where $\Delta_s$ is the Laplacian on the graph $\Gamma_1$, defined by (1.5). Furthermore, $\sqrt{\rho} > 0$, and $\rho > 0$ is the multiplication operator on $\ell^2(V_1)$ given by

$$(1.19) \quad (\rho f)(v) = \rho_v f(v), \quad \rho_v = \# \mathcal{Z}(v), \quad \mathcal{Z}(v) = (\{v\} + \mathbb{Z}^d) \cap V_1, \quad v \in V_1,$$

i.e., $\rho_v$ is the number of vertices from $V_1$ equivalent to $v$ with respect to the actions of the group $\mathbb{Z}^d$, $1 \leq \rho_v \leq \nu_1$, where $\nu_1 = \# V_1$ is the number of the vertices in $V_1$. Note that $\rho_v = 1$ for all $v \in V_o$.

2) The self-adjoint Dirichlet operator $H_\phi$ on $f \in \ell^2(V_1)$ is defined by

$$(1.20) \quad H_\phi f = H_1 f, \quad \text{where} \quad f|_{\partial V_1} = 0. $$

We will identify the Dirichlet operator $H_\phi$ on $f \in \ell^2(V_1)$ with the self-adjoint Dirichlet operator $H_\phi$ on $f \in \ell^2(V_o)$, since $f|_{\partial V_1} = 0$.

**Remark.** 1) The operator $\Delta_1$ is just the weighted Laplacian on $\ell^2(V_1)$.

2) Due to the boundary conditions $f|_{\partial V_1} = 0$ we call the operator $H_\phi$ the Dirichlet operator.

Denote the eigenvalues of the operators $H_\phi$, $\phi = 0, 1$, counted according to multiplicity, by

$$(1.21) \quad \lambda_0^0 \leq \lambda_2^0 \leq \ldots \leq \lambda_{\nu_\phi}^0, \quad \nu_\phi = \# V_\phi, \quad \phi = 0, 1.$$ 

We rewrite the sequence $q_1, \ldots, q_\nu$ defined by (1.13) in non-decreasing order

$$(1.22) \quad q_1^* \leq q_2^* \leq \ldots \leq q_\nu^*.$$ 

Here $q_1^* = q_{n_1}, q_2^* = q_{n_2}, \ldots, q_\nu^* = q_{n_\nu}$ for some distinct numbers $n_1, n_2, \ldots, n_\nu \in \mathbb{N}_\nu$.

**Theorem 1.1.** Each spectral band $\sigma_n(H)$ of the operator $H = \Delta + Q$ on the graph $\Gamma$ satisfies

$$(1.23) \quad \sigma_n(H) \subset J_n \cap \tilde{J}_n, \quad n \in \mathbb{N}_\nu,$$

where the intervals $J_n, \tilde{J}_n$ are given by

$$(1.24) \quad J_n = \begin{cases} [\lambda_n^1, \lambda_n^0], & n = 1, \ldots, \nu_0, \\
[\lambda_n^1, \lambda_n^* + 2\nu_+], & n = \nu_o + 1, \ldots, \nu,
\end{cases}$$

and

$$(1.25) \quad \tilde{J}_n = \begin{cases} [\lambda_n^*, \lambda_{n+\nu_0}^1], & n = 1, \ldots, \nu - \nu_0, \\
[\lambda_{n-\nu_0}^1, \lambda_{n+\nu_1-\nu}], & n = \nu - \nu_0 + 1, \ldots, \nu.
\end{cases}$$

**Remark.** 1) Due to Cattaneo correspondence [C97], Lledó and Post [LP08] considered the so-called normalized Laplacian $\hat{\Delta}$ on $\ell^2(V)$ given by $\hat{\Delta} = \nu^{-1/2} \Delta \nu^{-1/2}$, where $\nu^{1/2} > 0$ and $\nu > 0$ is the multiplication operator on $\ell^2(V)$ given by
$$(\kappa f)(v) = \kappa v f(v)$$.

They estimated the position of each band $\sigma_n(\Delta)$ for the normalized Laplacian $\Delta$ by $\sigma_n(\Delta) \subset J_n$, $n \in \mathbb{N}_\nu$, where the segments $J_n$ have the form similar to (1.24).

2) Let the graph $\Gamma$ be bipartite and regular of degree $\kappa_+$, i.e., each its vertex $v$ has the degree $\kappa_v = \kappa_+$. If $H = \Delta$, then $J_n = \zeta(J_{\nu-n+1})$ for each $n \in \mathbb{N}_\nu$, where $\zeta(z) = 2\kappa_+ - z$. Thus, in this case the estimate (1.23) has the form

$$\sigma_n(\Delta) \subset J_n \cap \zeta(J_{\nu-n+1}), \quad n \in \mathbb{N}_\nu.$$

3) Theorem 1.1 estimates the positions of the spectral bands in terms of eigenvalues of the operators $H_1$ and $H_\sigma$ on a fundamental domain $\Gamma_1$. Moreover, in some cases it allows us to detect the existence of gaps in the spectrum of the Schrödinger operator $H$. For example, for the graph shown in Figure 3 in the case when $H = \Delta$ the intervals $J_n \cap J_n$, $n \in \mathbb{N}_3$, are shown in Figure 3. The spectrum of the Laplacian $\Delta$ is also shown in this figure. As we can see, Theorem 1.1 detects precisely the second gap in the spectrum of the operator (for more details see Subsection 2.3).

**Figure 3.** a) A periodic graph $\Gamma$ and its fundamental domain $\Gamma_1$, the vertices of $\Gamma_1$ are big points (white and black); the edges of $\Gamma_1$ are marked by bold lines. The set of the inner vertices (black points) and the boundary (white points) are $V_o = \{v_1\}$ and $\partial V_1 = \{v_2, v_3, v_4, v_5, v_6, v_7\}$, respectively. b) The fundamental graph $\Gamma_F$; the vertices of $\Gamma_F$ are black. c) Eigenvalues of the operators $H_1$ and $H_\sigma$, the intervals $J_n$ and $\bar{J}_n$, $n \in \mathbb{N}_3$, and their intersections, the spectrum of the Laplacian $\Delta$.

4) Generally speaking, for distinct fundamental domains $\Gamma_1$ the operators $H_1, H_\sigma$, their eigenvalues and, consequently, the intervals $J_n, \bar{J}_n$ are different. We number
the fundamental domains $\Gamma_1^1, \Gamma_1^2, \ldots$. Thus, a more precise localization of the spectral bands of the Schrödinger operators $H$ on a periodic graph $\Gamma$ has the form

$$\sigma_n(H) \subset \bigcap_{\alpha} (J^o_{\alpha} \cap \tilde{J}^o_{\alpha}), \quad n \in \mathbb{N}_\nu,$$

where $J^o_{\alpha}, \tilde{J}^o_{\alpha}$ are the intervals, defined by (1.24), (1.25), for the fundamental domain $\Gamma_1^\alpha$. Sometimes, localization (1.26) gives the spectrum of the Schrödinger operators precisely (see Remark 1 after Example 4).

Now we estimate the total length of all spectral bands of $H$.

**Theorem 1.2.** i) The total length of all spectral bands $\sigma_n(H), \ n \in \mathbb{N}_\nu$, of $H$ satisfies

$$\sum_{n=1}^\nu |\sigma_n(H)| \leq \sum_{n=\nu_0+1}^\nu (q_n^* + 2\kappa_n - h_n) + \sum_{n=\nu_1+1}^{\nu_1} \lambda^1_n,$$

where $h_n = \rho_n(\kappa_n - \kappa_{nn} + q_n), \ \rho_n = \#Z(v_n)$, $\kappa_{nn}$ is the number of loops of the vertex $v_n$ on the graph $\Gamma$;

$$\sum_{n=1}^\nu |\sigma_n(H)| \leq \sum_{n=1}^{\nu - \nu_0} (\lambda^1_{\nu_1 - (\nu - \nu_0) + n} - \lambda^1_{\nu_1}).$$

ii) The numbers $\nu_0 = \#V_\phi, \ \phi = o, 1$ satisfy

$$0 \leq \nu_0 \leq \nu - 1, \quad \nu + d \leq \nu_1 \leq \#E_F + 1.$$

Moreover, equalities in (1.29) are achieved.

**Remark.** For the global estimate of the Lebesgue measure of the spectrum of Schrödinger operators $H$ it is enough to know the eigenvalues of the Neumann operator $H_1$.

2. **Proof of the main results**

2.1. **The Floquet matrix for the Schrödinger operator.** We need to introduce the two oriented edges $(u, v)$ and $(v, u)$ for each unoriented edge $(u, v) \in \mathcal{E}$: the oriented edge starting at $u \in V$ and ending at $v \in V$ will be denoted as the ordered pair $(u, v)$. We denote the sets of all oriented edges of the graph $\Gamma$ and the fundamental graph $\Gamma_F$ by $\mathcal{A}$ and $\mathcal{A}_F$, respectively.

We introduce an edge index, which is important to study the spectrum of Schrödinger operators on periodic graphs. For any $v \in V$ the following unique representation holds true:

$$v = [v] + \tilde{v}, \quad [v] \in \mathbb{Z}^d, \quad \tilde{v} \in V_F \subset [0, 1)^d.$$

In other words, each vertex $v$ can be represented uniquely as the sum of an integer part $[v] \in \mathbb{Z}^d$ and a fractional part $\tilde{v}$ that is a vertex of $V_F$ defined in (1.10). For any oriented edge $e = (u, v) \in \mathcal{A}$ we define the edge “index” $\tau(e)$ as the integer vector

$$\tau(e) = [v] - [u] \in \mathbb{Z}^d,$$

where due to (2.1) we have

$$u = [u] + \tilde{u}, \quad v = [v] + \tilde{v}, \quad [u], [v] \in \mathbb{Z}^d, \quad \tilde{u}, \tilde{v} \in V_F.$$
If $e = (u,v)$ is an oriented edge of the graph $\Gamma$, then by the definition of the fundamental graph there is an oriented edge $\tilde{e} = (\tilde{u}, \tilde{v})$ on $\Gamma_F$. For the edge $\tilde{e} \in A_F$ we define the edge index $\tau(\tilde{e})$ by

$$\tau(\tilde{e}) = \tau(e).$$

In other words, edge indices of the fundamental graph $\Gamma_F$ are induced by edge indices of the periodic graph $\Gamma$. The edge indices, generally speaking, depend on the choice of the coordinate origin $O$ and the periods $a_1, \ldots, a_d$ of the graph $\Gamma$. But in a fixed coordinate system the index of the fundamental graph edge is uniquely determined by (2.3), since

$$\tau(e + m) = \tau(e), \quad \forall (e, m) \in A \times \mathbb{Z}^d.$$

Edges with non-zero indices will be called bridges. For example, for the graph shown in Figure 3.1 the edges $(v_1, v_4), (v_1, v_5), (v_1, v_6), (v_1, v_7)$ are bridges. The bridges provide the connectivity of the periodic graph and the removal of all bridges disconnects the graph into infinitely many connected components.

The Schrödinger operator $H = \Delta + Q$ acting on $\ell^2(V)$ has the decomposition into a constant fiber direct integral (2.4), where the Floquet $\nu \times \nu$ matrix $H(\vartheta)$ has the form

$$H(\vartheta) = \Delta(\vartheta) + q, \quad q = \text{diag}(q_1, \ldots, q_\nu), \quad \forall \vartheta \in \mathbb{T}^d.$$

The Floquet matrix $\Delta(\vartheta) = \{\Delta_{jk}(\vartheta)\}_{j,k=1}^\nu$ for the Laplacian $\Delta$ is given by

$$\Delta_{jk}(\vartheta) = \sum_{e \in A} e^{i(\tau(e), \vartheta)}, \quad \forall (v_j, v_k) \in A_F,$$

see [KS13], where $\alpha_j$ is the degree of $v_j$, $\delta_{jk}$ is the Kronecker delta and $\langle \cdot, \cdot \rangle$ denotes the standard inner product in $\mathbb{R}^d$.

Now we need the following simple fact (see Theorem 4.3.1 in [HJ85]). Let $A, B$ be self-adjoint $\nu \times \nu$ matrices. Denote by $\lambda_1(A) \leq \ldots \leq \lambda_\nu(A)$, $\lambda_1(B) \leq \ldots \leq \lambda_\nu(B)$ the eigenvalues of $A$ and $B$, respectively, arranged in increasing order, counting multiplicities. Then we have

$$\lambda_n(A) + \lambda_1(B) \leq \lambda_n(A + B) \leq \lambda_n(A) + \lambda_\nu(B), \quad \forall n \in \mathbb{N}_\nu.$$

Inequalities (2.6) and the basic fact (1.6) give that the eigenvalues of the Floquet matrix $H(\vartheta)$ for the Schrödinger operator $H = \Delta + Q$, satisfy

$$q_n^* \leq \lambda_n(\vartheta) \leq q_n^* + 2\alpha_+, \quad \forall (\vartheta, n) \in \mathbb{T}^d \times \mathbb{N}_\nu,$$

$$\sigma_n(H) = \lambda_n(\mathbb{T}^d) \subset [q_n^*, q_n^* + 2\alpha_+], \quad \forall n \in \mathbb{N}_\nu.$$

### 2.2. Proof of the main results. In order to prove Theorem 1.1 we need the following lemma.

**Lemma 2.1.** The following inclusion holds true: $V_o \subset V_F$.

**Proof.** The proof is by contradiction. Let $u \in V_o$ and $u \notin V_F$. Then $v = u - m \in V_F \subset V_1$ for some $0 \neq m \in \mathbb{Z}^d$. First, we will show that $u$ and $v$ are not adjacent on $\Gamma$. Indeed, if $(u, v)_e \in \mathcal{E}$, then, due to the periodicity of $\Gamma$, $(u + m, u)_e \in \mathcal{E}$. Since $u \in V_o$, the incident to $u$ edges $(u, v)_e, (u + m, u)_e \in \mathcal{E}_1$. Thus, $\mathcal{E}_1$ contains $\mathbb{Z}^d$-equivalent edges, which contradicts the definition of the fundamental domain $\Gamma_1$ and we obtain that $u$ and $v$ are not adjacent on $\Gamma (u \sim v)$. Second, we will
show that \( \kappa^1_v = 0 \), that will contradict the connectivity of \( \Gamma_1 \) and complete the proof. Indeed, since \( u \in V_o \), all edges incident to \( u \) on \( \Gamma \) are contained in \( E_1 \). The vertices \( u \) and \( v \) are \( \mathbb{Z}^d \)-equivalent. Then all edges incident to \( v \) are \( \mathbb{Z}^d \)-equivalent to the corresponding edges incident to \( u \). Due to the definition of \( \Gamma_1 \) and the fact that \( u \sim v \), we conclude that \( E_1 \) does not contain any edges incident to \( v \). Thus, \( \kappa^1_v = 0 \). \( \square \)

Since \( V_o \subset V_F \), without loss of generality we may assume that the set \( V_o \) of the inner vertices of the graph \( \Gamma_1 = (V_1, E_1) \) has the form

\[
V_o = \{v_1, \ldots, v_{\nu_o}\}.
\]

We denote the equivalence classes from \( V_1/\mathbb{Z}^d \) by

\[
(2.8) \quad Z_j \equiv Z(v_j) = (\{v_j\} + \mathbb{Z}^d) \cap V_1, \quad j \in \mathbb{N}_\nu.
\]

The Neumann operator \( H_1 \) on the graph \( \Gamma_1 \) is equivalent to the \( \nu_1 \times \nu_1 \) self-adjoint matrix \( H_1 = \{H^1_{jk}\}_{j,k=1}^{\nu_1} \) given by

\[
(2.9) \quad H_1 = \Delta_1 + q^1, \quad q^1 = \text{diag}(q^1_1, \ldots, q^1_{\nu_1}),
\]

where \( q^1_k = q_j \), if \( v_k \in Z_j \), \( k \in \mathbb{N}_{\nu_1}, j \in \mathbb{N}_\nu \), and the matrix \( \Delta_1 = \{\Delta^1_{jk}\}_{j,k=1}^{\nu_1} \) has the form

\[
(2.10) \quad \Delta^1_{jk} = \sqrt{\rho_j \rho_k} (\kappa^1_j \delta_{jk} - \kappa^1_{jk}).
\]

Here \( \kappa^1_j \) is the degree of the vertex \( v_j \in V_1 \) on the graph \( \Gamma_1 \), \( \kappa^1_{jk} \geq 1 \) is the multiplicity of the edge \( (v_j, v_k) \in E_1 \) and \( \kappa^1_{jk} = 0 \) if \( (v_j, v_k) \notin E_1 \), \( \rho_j = \rho_v \) (see (1.19)).

The Dirichlet operator \( H_o \) is described by the \( \nu_o \times \nu_o \) self-adjoint matrix \( H_o = \{H^o_{jk}\}_{j,k=1}^{\nu_o} \) with entries

\[
(2.11) \quad H^o_{jk} = H^1_{jk} \quad \text{for all} \quad j, k \in \mathbb{N}_{\nu_o}.
\]

Recall that

\[
(2.12) \quad \kappa^1_j = \kappa_j \quad \text{and} \quad \rho_j = 1 \quad \text{for all} \quad j \in \mathbb{N}_{\nu_o}.
\]

**Proof of Theorem 1.1** We recall well-known facts. Denote by \( \lambda_1(A) \leq \ldots \leq \lambda_{\nu}(A) \) the eigenvalues of a self-adjoint \( \nu \times \nu \) matrix \( A \), arranged in increasing order, counting multiplicities. Each \( \lambda_n \) satisfies the minimax principle:

\[
(2.13) \quad \lambda_n(A) = \min_{S_n \subset \mathbb{C}^\nu} \max_{\|x\| = 1} \langle Ax, x \rangle,
\]

\[
(2.14) \quad \lambda_n(A) = \max_{S_{n-1} \subset \mathbb{C}^\nu} \min_{\|x\| = 1} \langle Ax, x \rangle,
\]

where \( S_n \) denotes a subspace of dimension \( n \) and the outer optimization is over all subspaces of the indicated dimension (see p. 180 in [HJ85]).

First, for each \( \vartheta \in \mathbb{T}^d \) we define the \( \nu \)-dimensional subspace \( Y_{\vartheta} \) of \( \mathbb{C}^{\nu_1} \) by

\[
(2.15) \quad Y_{\vartheta} = \{x = (x_k)^{\nu_1}_{k=1} \in \mathbb{C}^{\nu_1} : \forall k = \nu + 1, \ldots, \nu_1 \quad x_k = e^{i(v_k - v_j, \vartheta)} x_j, \quad \text{where} \quad j = j(k) \in \mathbb{N}_\nu \quad \text{is such that} \quad v_k \in Z_j \}.
\]
Note that \( j = j(k) \) in (2.13) is uniquely defined for each \( k = \nu + 1, \ldots, \nu_1 \). Let \( 1 \leq n \leq \nu \). Using (2.13) and (2.14) we write
\[
(2.16) \quad \lambda_j^1 = \min_{S_j \subseteq C^{\nu_1}} \max_{\|x\| = 1 \atop x \in S_j} \langle H_1 x, x \rangle \geq \min_{S_j \subseteq C^{\nu_1}} \max_{\|x\| = 1 \atop x \in S_j \cap Y_{\theta}} \langle H_1 x, x \rangle, \quad j = n + \nu_1 - \nu,
\]
\[
(2.17) \quad \lambda_n^1 = \min_{S_k \subseteq C^{\nu_1}} \max_{\|x\| = 1 \atop x \in S_k} \langle H_1 x, x \rangle \leq \max_{\|x\| = 1 \atop x \in S_k \cap Y_{\theta}} \min_{S_j \subseteq C^{\nu_1}} \langle H_1 x, x \rangle, \quad k = \nu_1 - n + 1,
\]
where \( S_j \) denotes a subspace of dimension \( j \). For \( x \in Y_{\theta} \) we have
\[
(2.18) \quad \langle H_1 x, x \rangle = \sum_{j,k=1}^{\nu_1} H_{jk} \bar{x}_j x_k = \sum_{j=1}^{\nu_1} (\rho_j \zeta_j^1 + q_j^1) |x_j|^2 - \sum_{j,k=1}^{\nu_1} \zeta_{jk}^1 \sqrt{\rho_j \rho_k} \bar{x}_j x_k,
\]
where
\[
(2.19) \quad \sum_{j=1}^{\nu_1} (\rho_j \zeta_j^1 + q_j^1) |x_j|^2 = \sum_{j=1}^{\nu_1} (\zeta_j + q_j) |x_j|^2 + \sum_{j=\nu_0+1}^{\nu} |x_j|^2 \sum_{v \in Z_j} (\rho_j \zeta_v^1 + q_j) \quad = \sum_{j=\nu_0+1}^{\nu} (\zeta_j + q_j) |x_j|^2 + \sum_{j=\nu_0+1}^{\nu} \rho_j (\zeta_j + q_j) |x_j|^2,
\]
\[
(2.20) \quad \sum_{j,k=1}^{\nu_1} \zeta_{jk}^1 \sqrt{\rho_j \rho_k} \bar{x}_j x_k = \sum_{j,k=1}^{\nu_1} \sqrt{\rho_j \rho_k} \sum_{e=(v_j, v_k) \in A_F} e^{i(\tau(e), \theta)} \bar{x}_j x_k.
\]
In (2.19) we have used the identities (2.12) and
\[
(2.21) \quad \sum_{v \in Z_j} \zeta_v^1 = \zeta_j,
\]
We introduce the new vector
\[
(2.22) \quad y = (y_j)_{j=1}^{\nu_1}; \quad y_j = \sqrt{\rho_j} x_j, \quad j \in \mathbb{N}_\nu.
\]
Since \( \rho_j = 1 \) for \( 1 \leq j \leq \nu_0 \), we have \( y_j = x_j, \ j \in \mathbb{N}_{\nu_0} \) and for \( x \in Y_{\theta} \) we obtain
\[
(2.23) \quad \|x\|^2 = \sum_{j=1}^{\nu_1} |x_j|^2 = \sum_{j=1}^{\nu_1} |x_j|^2 + \sum_{j=\nu_0+1}^{\nu} \rho_j |x_j|^2 = \sum_{j=1}^{\nu} |y_j|^2 = \|y\|^2.
\]
Combining (2.18) – (2.20) for \( x \in Y_{\theta}, (2.22) \) and the definition of \( H(\theta) \) in (2.4) we obtain
\[
(2.24) \quad \langle H_1 x, x \rangle = \sum_{j=1}^{\nu} (\zeta_j + q_j) |y_j|^2 - \sum_{j,k=1}^{\nu_1} \sum_{e=(v_j, v_k) \in A_F} e^{i(\tau(e), \theta)} \bar{y}_j y_k = \langle H(\theta)y, y \rangle.
\]
This, (2.16), (2.17), (2.23) and the minimax principle (2.13), (2.14) yield for \( 1 \leq n \leq \nu \):
\[
(2.25) \quad \lambda_{n+\nu_1-\nu}^1 \geq \min_{S_n \subseteq C^{\nu}} \max_{\|y\| = 1 \atop y \in S_n} \langle H(\theta)y, y \rangle = \lambda_n(\theta),
\]
\[
(2.26) \quad \lambda_n^1 \leq \max_{S_{\nu-n+1} \subseteq C^{\nu}} \min_{\|y\| = 1 \atop y \in S_{\nu-n+1}} \langle H(\theta)y, y \rangle = \lambda_n(\theta).
\]
Second, let \( X = \{ x \in \mathbb{C}^\nu : x_{\nu+1} = \ldots = x_\nu = 0 \} \) be the \( \nu_o \)-dimensional subspace of \( \mathbb{C}^\nu \) and let \( 1 \leq n \leq \nu_o \). Using (2.13) and (2.14) we write

\[
(2.27) \quad \lambda_j(\vartheta) = \min_{S_j \subset \mathbb{C}^\nu} \max_{\|x\| = 1} \langle H(\vartheta)x, x \rangle \geq \min_{S_j \subset \mathbb{C}^\nu} \max_{\|x\| = 1} \langle H(\vartheta)x, x \rangle, \quad j = n+\nu - \nu_o,
\]

\[
(2.28) \quad \lambda_n(\vartheta) = \max_{S_k \subset \mathbb{C}^\nu} \min_{\|x\| = 1} \langle H(\vartheta)x, x \rangle \leq \max_{S_k \subset \mathbb{C}^\nu} \min_{\|x\| = 1} \langle H(\vartheta)x, x \rangle, \quad k = \nu - n + 1.
\]

For \( x \in X \) we have

\[
(2.29) \quad \langle H(\vartheta)x, x \rangle = \sum_{j,k=1}^\nu H_{jk}(\vartheta) \bar{x}_j x_k = \sum_{j,k=1}^\nu H_{jk}^o \bar{x}_j x_k = \langle H_o x, x \rangle,
\]

\[
(2.30) \quad \|x\| = \|x\| = \sum_{j=1}^\nu |x_j|^2 = \sum_{j=1}^\nu |x_j|^2.
\]

Then for \( 1 \leq n \leq \nu_o \) we may rewrite the inequalities (2.27), (2.28) in the form

\[
(2.31) \quad \lambda_{n+\nu - \nu_o}(\vartheta) \geq \min_{S_n \subset \mathbb{C}^\nu} \max_{\|x\| = 1} \langle H_o x, x \rangle = \lambda_n^o,
\]

\[
(2.32) \quad \lambda_n(\vartheta) \leq \max_{S_n \subset \mathbb{C}^\nu} \min_{\|x\| = 1} \langle H_o x, x \rangle = \lambda_n^o.
\]

Combining (2.26) and (2.32) and using (2.7), we obtain for all \( \vartheta \in \mathbb{T}^d \)

\[
(2.33) \quad \lambda_n(\vartheta) \in [\lambda_n^1, \lambda_n^0] = J_n, \quad n = 1, \ldots, \nu_o,
\]

\[
(2.34) \quad \lambda_n(\vartheta) \in [\lambda_n^1, \lambda_n^1 + 2\lambda_+^1] = J_n, \quad n = \nu_o + 1, \ldots, \nu.
\]

Similarly, from (2.25) and (2.31) we obtain

\[
(2.35) \quad \lambda_n(\vartheta) \in [\lambda_n^0, \lambda_n^0 + 2\lambda_+^1] = \bar{J}_n, \quad n = 1, \ldots, \nu - \nu_o,
\]

\[
(2.36) \quad \lambda_n(\vartheta) \in [\lambda_n^1, \lambda_n^1 + 2\lambda_+^1] = \bar{J}_n, \quad n = \nu - \nu_o + 1, \ldots, \nu,
\]

for all \( \vartheta \in \mathbb{T}^d \). The relations (2.33) and (2.34) prove (1.23). \( \Box \)

**Proof of Theorem 1.2** i) First, we will prove the estimate (1.27). Let \( P \) be the projection onto \( L^2(\partial V_1) \). Using (1.21) we have

\[
\sum_{n=1}^\nu |\sigma_n(H)| \leq \sum_{n=1}^{\nu_o} (\lambda_n^1 - \lambda_n^1) + \sum_{n=\nu_o+1}^\nu (q_n^* + 2\lambda_+^1 - \lambda_n^1) = \text{Tr} \, H_o - \text{Tr} \, H_1
\]

\[
+ \sum_{n=\nu+1}^{\nu_o} \lambda_n^1 + \sum_{n=\nu_o+1}^\nu (q_n^* + 2\lambda_+) = \sum_{n=\nu+1}^{\nu_o} \lambda_n^1 + \sum_{n=\nu_o+1}^\nu (q_n^* + 2\lambda_+) - \text{Tr}(PH_1).
\]

Finally, applying (2.9), (2.10) to the diagonal entries of \( PH_1P \), we obtain

\[
(2.35) \quad \sum_{n=1}^\nu |\sigma_n(H)| \leq \sum_{n=\nu+1}^{\nu_o} \lambda_n^1 + \sum_{n=\nu_o+1}^\nu (q_n^* + 2\lambda_+) - \sum_{n=\nu_o+1}^\nu (\rho_n (x_n^1 - x_{nm}^1) + q_n^1)
\]

\[
= \sum_{n=\nu+1}^{\nu_o} \lambda_n^1 + \sum_{n=\nu_o+1}^\nu (q_n^* + 2\lambda_+ - \rho_n (x_n - x_{nm} + q_n)).
\]
Thus, the estimate (1.27) is proved.

Second, using (1.24) and (1.25) we have

\[
\sum_{n=1}^{\nu} |\sigma_n(H)| \leq \sum_{n=1}^{\nu} (\lambda_n^o - \lambda_n^1) + \sum_{n=\nu_0+1}^{\nu-\nu_o} (\lambda_n^1 - \lambda_{n-\nu_0}) + \sum_{n=\nu-\nu_o+1}^{\nu} (\lambda_n^1 - \lambda_{n-\nu_0})
\]

Thus, the estimate (1.28) is also proved.

ii) First, we will prove that 0 \leq \nu_0 \leq \nu - 1. We have 0 \leq \nu_0 and \nu_0 = 0 for some graphs (see, for example, Figure 2). Due to Lemma 2.21 \( V_0 \subseteq V_F \) and \( \nu_0 \leq \nu \). Assume that \( \nu_0 = \nu \), i.e., \( V_0 = V_F \). Then \( \sum_{v \in V_0} \chi_v^1 = \sum_{v \in V_0} \chi_v = \sum_{v \in V_F} \chi_v \). Using this and the fact that \( \partial V_1 = V_1 \setminus V_0 \neq \emptyset \) we obtain

\[
\# \mathcal{E}_1 = \frac{1}{2} \sum_{v \in V_1} \chi_v^1 > \frac{1}{2} \sum_{v \in V_0} \chi_v = \frac{1}{2} \sum_{v \in V_F} \chi_v = \# \mathcal{E}_F.
\]

Thus, \( \# \mathcal{E}_1 > \# \mathcal{E}_F \). From this we conclude that \( \Gamma_1 \) contains \( \mathbb{Z}^d \)-equivalent edges, which yields a contradiction. Therefore, \( \nu < \nu - 1 \) and \( \nu = \nu - 1 \) for some graphs (see Figure 2).

Second, we will show that \( \nu + d \leq \nu_1 \leq \# \mathcal{E}_F + 1 \). The connectivity of \( \Gamma_1 \) implies \( \nu_1 = \# V_1 \leq \# \mathcal{E}_1 + 1 \). The definition of the fundamental domain \( \Gamma_1 \) gives that \( \# \mathcal{E}_1 = \# \mathcal{E}_F \). Thus, \( \nu_1 \leq \# \mathcal{E}_F + 1 \). Since \( \mathbb{Z}^d \)-periodic graph \( \Gamma \) is connected, the fundamental domain \( \Gamma_1 \) has at least \( d \) bridges. Therefore, \( \# (V_1 \setminus V_F) \geq d \). This and \( V_F \subseteq V_1 \) yield \( \nu_1 \geq \nu + d \). The example in Figure 2 shows that \( \nu + d = \nu_1 = \# \mathcal{E}_F + 1 \).

2.3. Example 3. Consider the Laplacian \( H = \Delta \) on the periodic graph \( \Gamma \) shown in Figure 3a. The set of the fundamental graph vertices is \( V_F = \{ v_1, v_2, v_3 \} \). For each \( \vartheta = (\vartheta_1, \vartheta_2) \in \mathbb{T}^2 \) the matrix \( \Delta(\vartheta) \) defined by (2.3) has the form

\[
\Delta(\vartheta) = \begin{pmatrix}
6 & -\Delta_{12}(\vartheta) & -1 - e^{i\vartheta_2} \\
-\Delta_{12}(\vartheta) & 4 & 0 \\
-1 - e^{-i\vartheta_2} & 0 & 2
\end{pmatrix}, \quad \Delta_{12}(\vartheta) = (1 + e^{i\vartheta_1})(1 + e^{i\vartheta_2})
\]

The characteristic polynomial of \( \Delta(\vartheta) \) is given by

\[
\det(\Delta(\vartheta) - \lambda \mathbb{I}_3) = -\lambda^3 + 12\lambda^2 + 2(2c_1c_2 + 2c_1 + 3c_2 - 19)\lambda - 4(2c_1c_2 + 2c_1 + 4c_2 - 8),
\]

\( \mathbb{I}_3 \) is the \( 3 \times 3 \) identity matrix, \( c_1 = \cos \vartheta_1, \ c_2 = \cos \vartheta_2 \). The spectrum of the Laplacian \( \Delta \) on the periodic graph \( \Gamma \) consists of three bands:

\[
\sigma_1 = [0; 2], \quad \sigma_2 \approx [2.5; 4], \quad \sigma_3 \approx [6; 9.5].
\]
The fundamental domain $\Gamma_1 = (V_1, E_1)$ shown in Figure 3a has the vertex set $V_1$ given by

$$V_1 = \{v_1, v_2, v_3, v_4 = v_2 + a_1, v_5 = v_2 + a_1 + a_2, v_6 = v_3 + a_2, v_7 = v_2 + a_2\}.$$

The set of the inner vertices $V_o$ and the boundary $\partial V_1$ of $\Gamma_1$ have the form

$$V_o = \{v_1\}, \quad \partial V_1 = \{v_2, v_3, v_4, v_5, v_6, v_7\}.$$

The matrices $H_1$ and $H_o$, defined by (2.9) – (2.11), in this case have the form

$$H_1 = \begin{pmatrix} 6 & A \end{pmatrix}^T \begin{pmatrix} A & D \end{pmatrix}, \quad A = -\begin{pmatrix} 2 & \sqrt{2} & 2 & \sqrt{2} & 2 \end{pmatrix},$$

$$D = \text{diag}(4, 2, 4, 2, 4), \quad H_o = 6.$$

The spectra of the operators $H_1$ and $H_o$ are

$$\sigma(H_1) \approx \{0; 2; 2.5; 4; 4; 4.95\}, \quad \sigma(H_o) = \{6\}.$$

Thus, the intervals $J_n$ and $\tilde{J}_n$ defined by (1.24), (1.25) and their intersections $J_n \cap \tilde{J}_n$, $n \in \mathbb{N}_3$, have the form

$$J_1 = [0; 6], \quad \tilde{J}_1 = [0, 4], \quad \sigma_1 = [0; 2] \subset J_1 \cap \tilde{J}_1 = J_1 = [0; 4],$$

$$J_2 = [2; 12], \quad \tilde{J}_2 = [0; 4], \quad \sigma_2 \approx [2.5; 4] \subset J_2 \cap \tilde{J}_2 = [2; 4],$$

$$J_3 \approx [2.5; 12], \quad \tilde{J}_3 \approx [6; 9.5], \quad \sigma_3 \approx [6; 9.5] = J_3 \cap \tilde{J}_3 = J_3.$$

**Remark.** 1) Theorem 1.1 determines the existence of the second spectral gap (see Figure 3c). The intersection of the intervals $J_n$ and $\tilde{J}_n$, $n = 1, 2, 3$, gives more
precise estimates of the spectral band \( \sigma_n(H) \) than one interval \( J_n \). Moreover, for \( n = 2, 3 \) the estimate \( \sigma_n(H) \subset J_n \) gives the upper bound \( \lambda_n(\vartheta) \leq 2\chi_+ = 12 \) that is trivial. But using (1.23) we obtain more accurate estimates for the spectral bands. Note that the last spectral band and the last gap are detected precisely, but the first band is estimated too roughly and the first spectral gap is not detected.

2) For the graph shown in Figure 3, the estimates (1.27), (1.28) have the form

\[
\sum_{n=1}^{3} |\sigma_n(H)| \leq \sum_{n=2}^{3} (12 - h_n) + \sum_{n=4}^{7} \lambda_n^1 \approx 25.5,
\sum_{n=1}^{3} |\sigma_n(H)| \leq \sum_{n=1}^{2} (\lambda_{5+n}^1 - \lambda_n^1) \approx 11.5.
\]

Thus, the second estimate is much better than the first one. Finally, we note that (2.37) yields

\[
\sum_{n=1}^{3} |\sigma_n(H)| \approx (2 - 0) + (4 - 2.5) + (9.5 - 6) = 7.0.
\]

![Diagram](image)

**Figure 5.** a) The same periodic graph \( \Gamma \) and another fundamental domain \( \Gamma_1 \). The set of the inner vertices (black points) and the boundary (white points) are \( V_o = \{v_1\} \) and \( \partial V_1 = \{v_2, v_3, v_4, v_5\} \), respectively. b) The fundamental graph \( \Gamma_F \); the vertices of \( \Gamma_F \) are black. c) Eigenvalues of the operators \( H_1 \) and \( H_o \), the intervals \( J_n \) and \( \overline{J}_n \), \( n \in \mathbb{N}_3 \), and their intersections, the spectrum of the Laplacian \( \Delta \).

**Example 4.** We can choose the fundamental graph \( \Gamma_1 \) for the periodic graph \( \Gamma \) in Example 3 by another way as shown in Figure 5b. For this finite graph \( \Gamma_1 = (V_1, \mathcal{E}_1) \) we have

\[
V_1 = \{v_1, v_2, v_3, v_4 = v_2 + a_2, v_5 = v_3 + a_1\}, \quad V_o = \{v_1\}, \quad \partial V_1 = \{v_2, v_3, v_4, v_5\}.
\]
The matrices $H_1$ and $H_o$, defined by (2.9) – (2.11), have the form

$$H_1 = \begin{pmatrix} 2 & -\sqrt{2} & 0 & -\sqrt{2} & 0 \\ -\sqrt{2} & 6 & -2 & 0 & -2 \\ 0 & -2 & 4 & -2 & 0 \\ -\sqrt{2} & 0 & -2 & 6 & -2 \\ 0 & -2 & 0 & -2 & 4 \end{pmatrix}, \quad H_o = 2.$$  

The spectra of the operators $H_1$ and $H_o$ are

$$\sigma(H_1) \approx \{ 0; 2.5; 4; 6; 9.5 \}, \quad \sigma(H_o) = \{ 2 \}.  

Thus, the intervals $J_n$ and $\tilde{J}_n$ defined by (1.24), (1.25) and their intersections $J_n \cap \tilde{J}_n$, $n \in \mathbb{N}_3$, have the form

$$J_1 = [0; 2], \quad \tilde{J}_1 = [0, 4], \quad \sigma_1 = [0; 2] = J_1 \cap \tilde{J}_1 = J_1,$$

$$J_2 \approx [2.5; 12], \quad \tilde{J}_2 = [0; 6], \quad \sigma_2 \approx [2.5; 4] \subset J_2 \cap \tilde{J}_2 \approx [2.5; 6],$$

$$J_3 = [4; 12], \quad \tilde{J}_3 \approx [2; 9.5], \quad \sigma_3 \approx [6; 9.5] \subset J_3 \cap \tilde{J}_3 \approx [4; 9.5].$$

Remark. 1) Due to Remark 4 after Theorem 1.1, formulas (2.38), (2.39) give

$$\sigma_1 = [0; 2] \subset [0; 4] \cap [0; 2] = [0; 2],$$

$$\sigma_2 \approx [2.5; 4] \subset [2; 4] \cap [2.5; 6] = [2.5; 4],$$

$$\sigma_3 \approx [6; 9.5] \subset [6; 9.5] \cap [4; 9.5] = [6; 9.5].$$

Thus, in the considered example, the use of only 2 fundamental domains gives the spectrum of the Laplacian precisely.

2) For the graph shown in Figure 5a the estimates (1.27), (1.28) have the form

$$\sum_{n=1}^{3} |\sigma_n(H)| \leq \sum_{n=2}^{3} (12 - h_n) + \sum_{n=4}^{5} \lambda_1^n \approx 19.5, \quad \sum_{n=1}^{3} |\sigma_n(H)| \leq \sum_{n=1}^{2} (\lambda_3^{1+n} - \lambda_1^n) \approx 13.$$

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