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 obtain a localization of spectral bands in terms of eigenvalues of Dirichlet and Neumann operators on a finite graph, which is constructed from the fundamental cell of the periodic graph. The proof is based on the Floquet decomposition of Schrödinger operators and the minimax principle.

1. Introduction and main result

Operators on periodic graphs are of interest due to their applications to problems of physics and chemistry. They are used to describe and to study properties of different periodic media, including nanomedia. We consider Schrödinger operators with periodic potentials on \( \mathbb{Z}^d \)-periodic discrete graphs, \( d \geq 2 \). 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 \( Q \) in \( \mathbb{R}^d \) 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. For the case of periodic graphs we know only two papers about estimates of spectrum and gaps:

1. Lledó and Post [LP08] considered Laplacians on metric graphs. In this case they determined estimates (the so-called eigenvalue bracketing) using various types of boundary conditions at the vertices. Via an explicit Cattaneo correspondence [C97] of the equilateral metric and discrete graph spectra they carry over these estimates from the metric graph Laplacian to the normalized Laplacian on the discrete graph. 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 [LP08]).

2. Korotyaev and Saburova [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 estimate the position of bands of discrete Schrödinger operators on periodic graphs. Here even for the Laplacian the Lledó-Post result [LP08] does not work, since our Laplacian is not normalized and the Cattaneo correspondence between the spectra of Laplacians on discrete and metric graphs treated in [LP08] does not hold true. We estimate directly...
spectral band positions of discrete Schrödinger operators in terms of eigenvalues of Dirichlet and Neumann operators on a finite graph, which is constructed from the fundamental cell of the periodic graph. These estimates in some cases allow to determine the existence of gaps in the spectrum of Schrödinger operators. Note that even for Laplacians it is new.

### 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 unordered 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 $\mathbb{R}^d$ such that $\Gamma$ is invariant under translations through the vectors $a_1, \ldots, a_d$:

   $$\Gamma + a_s = \Gamma, \quad \forall s \in \mathbb{N}_d = \{1, \ldots, d\}.$$ 

The vectors $a_1, \ldots, a_d$ are called the periods of $\Gamma$.

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 square summable 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 $f \in \ell^2(V)$ by

$$(\Delta f)(v) = \sum_{(v, u) \in E} (f(v) - f(u)), \quad v \in V. \quad (1.1)$$

We recall the basic facts (see [Mc94], [M92], [MW89]) for both finite and periodic graphs: *the point 0 belongs to the spectrum $\sigma(\Delta)$ and $\sigma(\Delta)$ is contained in $[0, 2\kappa_+)$, i.e.,*

$$0 \in \sigma(\Delta) \subset [0, 2\kappa_+), \quad \text{where } \kappa_+ = \sup_{v \in V} \deg v < \infty. \quad (1.2)$$

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

$$H = \Delta + Q, \quad (1.3)$$

$$Q f(v) = Q(v) f(v), \quad \forall v \in V, \quad (1.4)$$

where we assume that the potential $Q$ is real valued and satisfies

$$Q(v + \tilde{a}_s) = Q(v), \quad \forall (v, s) \in V \times \mathbb{N}_d,$$

for some linearly independent integer vectors $\tilde{a}_1, \ldots, \tilde{a}_d \in \mathbb{Z}^d$ (in the basis $a_1, \ldots, a_d$). The vectors $\tilde{a}_1, \ldots, \tilde{a}_d$ are called *the periods of the potential* $Q$. Since the periods $\tilde{a}_1, \ldots, \tilde{a}_d$ of the potential are also periods of the periodic graph, we may assume that the periods of the potential are the same as the periods of the graph.
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 \( \nu = \#V_F \) is the number of vertices of \( \Gamma_F \).

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

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

\( \mathbb{T}^d = \mathbb{R}^d/(2\pi\mathbb{Z})^d \), 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 \( \Delta(\vartheta) = \{\Delta_{jk}(\vartheta)\}_{j,k=1}^\nu \) for the Laplacian \( \Delta \) is given by (2.3). 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

\[
\sigma_n = \sigma_n(H) = [\lambda_n^-, \lambda_n^+] = \lambda_n(\mathbb{T}^d), \quad \lambda_n^+ = \max_{\vartheta \in \mathbb{T}^d} \lambda_n(\vartheta), \quad \lambda_n^- = \min_{\vartheta \in \mathbb{T}^d} \lambda_n(\vartheta).
\]

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-degenerated intervals, and \( \sigma_{fb}(H) \) is the set of all flat bands (eigenvalues of infinite multiplicity). An open interval between two neighboring non-degenerated spectral bands is called a spectral gap.
1.3. Localization of spectral bands for Schrödinger operators. In order to formulate estimates of spectral band positions we define two operators on a finite graph \( \Gamma_N = (V_N, E_N) \) with a vertex set \( V_N \) and an edge set \( E_N \). This graph is introduced by the following way. Denote by \( E^m_N \) the set of all edges of \( \Gamma \) connecting the vertices from \( V_F \), defined by (1.6). An edge connecting a vertex from \( V_F \) with a vertex from \( V \setminus V_F \) is called a bridge. Denote by \( B \) the set of all bridges. Since \( \mathbb{Z}^d \)-periodic graph \( \Gamma \) is connected, the number \( \beta = \# B \) of all bridges of \( \Gamma \) depends on the choice of the coordinate origin \( O \) and satisfies \( 2d \leq \beta \). Due to periodicity of the graph the set \( B \) consists of pairs of equivalent to each other (with respect to the action of the group \( \mathbb{Z}^d \)) bridges. We take one bridge from each pair and denote the obtained set of bridges by \( B_N \). The finite graph \( \Gamma_N = (V_N, E_N) \) is the edge-induced subgraph of \( \Gamma \), its edge set is \( E_N = E^m_N \cup B_N \) and its vertex set \( V_N \) consists of all ends of edges of \( E_N \), i.e.,

\[
E_N = E^m_N \cup B_N, \quad V_N = V_F \cup \{ u \in V : (u, v) \in B_N, v \in V_F \}.
\]

Let \( \nu_v = \text{deg} v \) be the degree of the vertex \( v \in V_N \) on the graph \( \Gamma_N \). A vertex \( v \in V_N \) will be called an inner vertex of \( \Gamma_N \), if \( \nu_v = \nu_v^N \), i.e., if all its adjacent (neighbor) vertices from \( V \) also belong to the graph \( \Gamma_N \). Denote by \( V_D \) the set of all inner vertices of \( \Gamma_N \). Let \( \nu_{\partial} = \# \partial v \) be the number of the vertices in \( \partial v \), \( \phi = D, N \). We define a boundary \( \partial V_N \) of \( \Gamma_N \) by the standard identity:

\[
\partial V_N = V_N \setminus V_D.
\]

**Figure 1.** a) A periodic graph \( \Gamma \) and its finite graph \( \Gamma_N \), the vertices of the graph \( \Gamma_N \) are black; the edges of \( \Gamma_N \) are marked by bold lines. The set of the inner vertices and the boundary are \( V_D = \{ v_1 \} \) and \( \partial V_N = \{ v_2, v_3, v_4, v_5, v_6, v_7 \} \), respectively. b) Eigenvalues of the operators \( H_N \) and \( H_D \), the intervals \( J_n \) and \( J_n \), \( n \in \mathbb{N} \), and their intersections, the spectrum of the Laplacian \( \Delta \).
Example. For $\mathbb{Z}^2$-periodic graph shown in Fig. 1, the set $V_F$ consists of the vertices \{v_1, v_2, v_3\}. The finite graph $\Gamma_N = (V_N, E_N)$ has the vertex set $V_N$ given by
\[ V_N = \{v_1, v_2, v_3, v_4 = v_2 + a_1, v_5 = v_2 - a_2, v_6 = v_3 - a_2, v_7 = v_2 + a_1 - a_2\}. \]
The set of the inner vertices $V_D$ and the boundary $\partial V_N$ of $\Gamma_N$ have the form
\[ V_D = \{v_1\}, \quad \partial V_N = \{v_2, v_3, v_4, v_5, v_6, v_7\}. \]

On the finite graph $\Gamma_N$ we define two self-adjoint operators $H_N$ and $H_D$: 1) The Neumann operator $H_N$ on $\ell^2(V_N)$ is defined by
\[ H_N = \Delta_N + Q, \tag{1.15} \]
where
\[ (\Delta_N f)(v) = \rho_v \kappa_v^{N} f(v) - \sqrt{\rho_v} \sum_{(v, u) \in E_N} \sqrt{\rho_u} f(u), \quad v \in V_N, \quad f \in \ell^2(V_N), \tag{1.16} \]
\[ \rho_v = \# V_v, \quad V_v = \{(v) + \mathbb{Z}^d\} \cap V_N, \quad v \in V_N, \tag{1.17} \]
i.e., $\rho_v$ is the number of vertices from $V_N$ equivalent to $v$ with respect to the action of the group $\mathbb{Z}^d$.

2) The Dirichlet operator $H_D$ on $f \in \ell^2(V_N)$ is also defined by (1.15), but with the Dirichlet boundary conditions $f(v) = 0$ for all $v \in \partial V_N$. We will identify the Dirichlet operator $H_D$ on $f \in \ell^2(V_N)$ with the Dirichlet operator $H_D$ on $f \in \ell^2(V_D)$, since $f(v) = 0$ for all $v \in \partial V_N$.

Denote the eigenvalues of the operators $H_\phi, \phi = D, N$, counted according to multiplicity, by
\[ \lambda^\phi_1 \leq \lambda^\phi_2 \leq \ldots \leq \lambda^\phi_{\nu_\phi}, \quad \nu_\phi = \# V_\phi, \quad \phi = D, N. \tag{1.18} \]
We rewrite the sequence $q_1, \ldots, q_{\nu}$ define by (1.9) in nondecreasing order
\[ q_1^* \leq q_2^* \leq \ldots \leq q_{\nu}^* . \tag{1.19} \]
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
\[ \sigma_n(H) \subset J_n \cap \tilde{J}_n, \quad n \in \mathbb{N}_\nu, \tag{1.20} \]
where the intervals $J_n, \tilde{J}_n$ are given by
\[ J_n = \begin{cases} [\lambda^n_1, \lambda^n_D], & n = 1, \ldots, \nu_D, \\ [\lambda^n_1, q^n_* + 2\kappa_+^N], & n = \nu_D + 1, \ldots, \nu, \end{cases} \tag{1.21} \]
and
\[ \tilde{J}_n = \begin{cases} [q^n_* - \nu N - \nu + 1, \lambda^n_{\nu + \nu N - \nu}], & n = 1, \ldots, \nu - \nu_D, \\ [\lambda^n_{\nu - \nu N + \nu D}, \lambda^n_{1 + \nu N - \nu}], & n = \nu - \nu_D + 1, \ldots, \nu. \end{cases} \tag{1.22} \]

**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 $\hat{\Delta} = \chi \Delta \chi$, where $\chi$ is the multiplication operator on $\ell^2(V)$ given by $(\chi f)(v) = \kappa_v^{N+\frac{1}{2}} f(v)$ and $\kappa_+^N > 0$. They estimated the position of the band $\sigma_n(\hat{\Delta})$ for the normalized Laplacian $\hat{\Delta}$ by $\sigma_n(\hat{\Delta}) \subset \tilde{J}_n$, $n \in \mathbb{N}_\nu$, where the segments $\tilde{J}_n$ have the form similar to $J_n$ from (1.21).
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 $\tilde{J}_n = \zeta(J_n)$ for each $n \in \mathbb{N}_\nu$, where $\zeta(z) = 2\kappa_+ - z$. Thus, in this case the estimate (1.20) has the form

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

3) Theorem 1.1 estimates the positions of the spectral bands in terms of eigenvalues of the operators $H_N$ and $H_D$ on the finite graph $\Gamma_N$. Moreover, in some cases it allows to detect the existence of gaps in the spectrum of the Schrödinger operator $H$. For example, for the graph shown in Fig.1, in the case when $H = \Delta$ the intervals $J_n \cap \tilde{J}_n$, $n \in \mathbb{N}_\nu$, are shown in Fig.1b. 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).

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

$$\sum_{n=1}^{\nu} |\sigma_n(H)| \leq \sum_{n=\nu+1}^{\nu+\nu_D} (q_n^* + 2\kappa_+ - h_n) + \sum_{n=\nu+1}^{\nu+\nu_N} \lambda_n^N,$$  

(1.23)

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

$$\sum_{n=1}^{\nu} |\sigma_n(H)| \leq \sum_{n=1}^{\nu+\nu_D} (\lambda_n^N - (\nu+\nu_D) + n - \lambda_n^N).$$  

(1.24)

ii) The numbers $\nu_\phi = \#V_\phi$, $\phi = D, N$ satisfy

$$0 \leq \nu_D \leq \nu - 1, \quad \nu + d \leq \nu_N \leq \nu + \frac{\beta}{2},$$  

(1.25)

where $\beta = \#B$ is the number of the bridges of $\Gamma$. Moreover, the boundaries of the inequalities (1.25) 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 $H_N$.

2. **Proof of the main result**

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:

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

(2.1)

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 (1.6). For any oriented edge $e = (u, v) \in \mathcal{A}$ we define the edge ”index” $\tau(e)$ as the integer vector

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

(2.2)

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 \( \tilde{e} \in \mathcal{A}_F \) we define the edge index \( \tau(\tilde{e}) \) by
\[
\tau(\tilde{e}) = \tau(e).
\]
(2.3)

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 \( O \). But in a fixed coordinate system the index of the fundamental graph edge is uniquely determined by \( \tau(\tilde{e}) \), since
\[
\tau(e + m) = \tau(e), \quad \forall (e, m) \in \mathcal{A} \times \mathbb{Z}^d.
\]

Note that all bridges of the graph \( \Gamma \) have nonzero indices.

The Schrödinger operator \( H = \Delta + Q \) acting on \( \ell^2(V) \) has the decomposition into a constant fiber direct integral \( \ell^2(\nu) \), where the Floquet \( \nu \times \nu \) matrix \( H(\vartheta) \) has the form
\[
H(\vartheta) = \Delta(\vartheta) + \kappa, \quad \kappa = \text{diag}(q_1, \ldots, q_\nu), \quad \forall \vartheta \in \mathbb{T}^d.
\]

(2.4)

The Floquet matrix \( \Delta(\vartheta) = \{\Delta_{jk}(\vartheta)\}_{j,k=1}^\nu \) for the Laplacian \( \Delta \) is given by
\[
\Delta_{jk}(\vartheta) = \kappa_j \delta_{jk} - \left\{ \begin{array}{ll}
\sum_{\vartheta = (v_j, v_k) \in \mathcal{A}_F} e^{i(\tau(\vartheta), \vartheta)} & \text{if } (v_j, v_k) \in \mathcal{A}_F \\
0 & \text{if } (v_j, v_k) \notin \mathcal{A}_F
\end{array} \right.,
\]
(2.5)

see [KS13], where \( \kappa_n \) 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
\[
\lambda_n(A) + \lambda_1(B) \leq \lambda_n(A + B) \leq \lambda_n(A) + \lambda_\nu(B) \quad \forall n \in \mathbb{N}_\nu.
\]

(2.6)

Inequalities (2.6) and the basic fact (1.2) give that the eigenvalues of the Floquet matrix \( H(\vartheta) \) for the Schrödinger operator \( H = \Delta + Q \), satisfy
\[
\kappa_n \leq \lambda_n(\vartheta) \leq \kappa_n + 2\kappa_+, \quad \forall (\vartheta, n) \in \mathbb{T}^d \times \mathbb{N}_\nu,
\]
\[
\sigma_n(H) = \lambda_n(\mathbb{T}^d) \subset [\kappa_n, \kappa_n + 2\kappa_+], \quad \forall n \in \mathbb{N}_\nu.
\]

(2.7)

2.2. Proof of the main result. Without loss of generality we may assume that the set of inner vertices \( V_D \) of the graph \( \Gamma_N = (V_N, \mathcal{E}_N) \) has the form
\[
V_D = \{v_1, \ldots, v_{\nu_D}\}.
\]

We denote the equivalence classes from \( V_N/\mathbb{Z}^d \) by
\[
V_j = (\{v_j\} + \mathbb{Z}^d) \cap V_N, \quad j \in \mathbb{N}_\nu.
\]

(2.8)

The Neumann operator \( H_N \) on the graph \( \Gamma_N \) is equivalent to the \( \nu_N \times \nu_N \) self-adjoint matrix \( H_N = \{H_{jk}^N\}_{j,k=1}^{\nu_N} \) given by
\[
H_N = \Delta_N + q_N, \quad q_N = \text{diag}(q_1^N, \ldots, q_\nu^N),
\]

(2.9)

where \( q_k^N \equiv q_j \), if \( v_k \in V_j, k \in \mathbb{N}_\nu, j \in \mathbb{N}_\nu \), and the matrix \( \Delta_N = \{\Delta_{jk}^N\}_{j,k=1}^{\nu_N} \) has the form
\[
\Delta_{jk}^N = \sqrt{\rho_j \rho_k} (\kappa_j^N \delta_{jk} - \kappa_{jk}^N).
\]

(2.10)
Here $x_j^N$ is the degree of the vertex $v_j \in V_N$ on the graph $\Gamma_N$, $x_j^N \geq 1$ is the multiplicity of the edge $(v_j, v_k) \in E_N$ and $x_j^N = 0$ if $(v_j, v_k) \notin E_N$, $\rho_j = |V_j|$ is the number of vertices in $V_j$.

The Dirichlet operator $H_D$ is described by the $\nu_D \times \nu_D$ self-adjoint matrix $H_D = \{H_{jk}^D\}_{j,k=1}^{\nu_D}$ with entries

$$H_{jk}^D = H_{jk}^N \quad \text{for all } j, k \in \mathbb{N}_{\nu_D}. \quad (2.11)$$

Recall that

$$x_j^N = x_j \quad \text{and} \quad \rho_j = 1 \quad \text{for all } j \in \mathbb{N}_{\nu_D}. \quad (2.12)$$

**Proof of Theorem 1.1** For each $\vartheta \in \mathbb{T}^d$ we define the $\nu$-dimensional subspace $Y_\vartheta$ of $\mathbb{C}^{\nu_N}$ by

$$Y_\vartheta = \{ x = (x_k)_{k=1}^{\nu_N} \in \mathbb{C}^{\nu_N} : \forall k = \nu + 1, \ldots, \nu_N \quad x_k = e^{i(v_k - v_j, \vartheta)} x_j, \quad \text{where } j = j(k) \in \mathbb{N}_\nu \text{ is such that } v_k \in V_j \}. \quad (2.13)$$

Note that $j = j(k)$ in (2.13) is uniquely defined for each $k = \nu + 1, \ldots, \nu_N$.

Let $X$ be the $\nu_D$-dimensional subspace of $\mathbb{C}^{\nu}$, defined by

$$X = \{ x \in \mathbb{C}^\nu : x_{\nu_D+1} = \ldots = x_\nu = 0 \}. \quad (2.14)$$

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:

$$\lambda_n(A) = \min_{S_n \subset \mathbb{C}^{\nu_N}} \max_{x \in S_n} \langle Ax, x \rangle, \quad (2.15)$$

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 [13]).

First, let $1 \leq n \leq \nu$. Using (2.14) and (2.15) we write

$$\lambda_j^N = \min_{S_j \subset \mathbb{C}^{\nu_N}} \max_{x \in S_j} \langle H_N x, x \rangle \geq \min_{S_j \subset \mathbb{C}^{\nu_N}} \max_{x \in S_j / Y_\vartheta} \langle H_N x, x \rangle, \quad j = n + \nu_N - \nu, \quad (2.16)$$

$$\lambda_n = \max_{S_k \subset \mathbb{C}^{\nu_N}} \min_{x \in S_k / Y_\vartheta} \langle H_N x, x \rangle \leq \max_{S_k \subset \mathbb{C}^{\nu_N}} \min_{x \in S_k} \langle H_N x, x \rangle, \quad k = \nu_N - n + 1, \quad (2.17)$$

where $S_j$ denotes a subspace of dimension $j$. For $x \in Y_\vartheta$ we have

$$\langle H_N x, x \rangle = \sum_{j,k=1}^{\nu_N} H_{jk}^N \bar{x}_j x_k = \sum_{j=1}^{\nu_N} (\rho_j x_j^N + q_j^N) |x_j|^2 - \sum_{j,k=1}^{\nu_N} x_{jk} N \sqrt{\rho_j \rho_k} \bar{x}_j x_k, \quad (2.18)$$

where

$$\sum_{j=1}^{\nu_N} (\rho_j x_j^N + q_j^N) |x_j|^2 = \sum_{j=1}^{\nu_D} (\rho_j + q_j) |x_j|^2 + \sum_{j=\nu_D+1}^{\nu} |x_j|^2 \sum_{v \in V_j} \rho_j (x_v^N + q_j)$$

$$= \sum_{j=1}^{\nu_D} (\rho_j + q_j) |x_j|^2 + \sum_{j=\nu_D+1}^{\nu} \rho_j (x_j + q_j) |x_j|^2, \quad (2.19)$$
\[
\sum_{j,k=1}^{\nu_N} \zeta_{jk}^N \sqrt{\rho_j \rho_k} \bar{x}_j x_k = \sum_{j,k=1}^{\nu} \sqrt{\rho_j \rho_k} \sum_{e=(v_j, v_k) \in A_F} e^{i \langle \tau(e), \vartheta \rangle} \bar{x}_j x_k. \tag{2.20}
\]

In (2.19) we have used the identities (2.12) and

\[
\sum_{v \in V_j} \zeta_v^N = \zeta_j. \tag{2.21}
\]

We introduce the new vector

\[
y = (y_j)_{j=1}^{\nu}, \quad y_j = \sqrt{\rho_j} x_j, \quad j \in \mathbb{N}_\nu. \tag{2.22}
\]

Since \( \zeta_j = 1 \) for \( 1 \leq j \leq \nu_D \), we have \( y_j = x_j, \ j \in \mathbb{N}_{\nu_D} \), and, using (2.21), for \( x \in \mathfrak{V}_\theta \) we have

\[
\|x\|^2 = \sum_{j=1}^{\nu} |x_j|^2 \leq \sum_{j=1}^{\nu} |x_j|^2 + \sum_{j=\nu_D+1}^{\nu} \rho_j |x_j|^2 = \sum_{j=1}^{\nu} |y_j|^2 = \|y\|^2. \tag{2.23}
\]

Combining (2.18) – (2.20) for \( x \in \mathfrak{V}_\theta \), (2.22) and the definition of \( H(\vartheta) \) in (2.3) we obtain

\[
\langle H_N x, x \rangle = \sum_{j=1}^{\nu} \langle x_j + q_j \rangle |y_j|^2 - \sum_{j,k=1}^{\nu} \sum_{e=(v_j,v_k) \in A_F} e^{i \langle \tau(e), \vartheta \rangle} \bar{y}_j y_k = \langle H(\vartheta)y, y \rangle. \tag{2.24}
\]

This, (2.16), (2.17), (2.23) and the minimax principle (2.14), (2.15) yield for \( 1 \leq n \leq \nu \):

\[
\lambda_{n+\nu-N}^N \geq \min_{S_n \subset \mathbb{C}^\nu} \max_{\|y\|=1} \langle H(\vartheta)y, y \rangle = \lambda_n(\vartheta), \tag{2.25}
\]

\[
\lambda_{n}^N \leq \max_{S_{\nu-n+1} \subset \mathbb{C}^\nu} \min_{\|x\|=1} \langle H(\vartheta)x, x \rangle = \lambda_n(\vartheta). \tag{2.26}
\]

Second, let \( 1 \leq n \leq \nu_D \). Using (2.14) and (2.15) we write

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

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

For \( x \in \mathfrak{X} \) we have

\[
\langle H(\vartheta)x, x \rangle = \sum_{j,k=1}^{\nu} H_{jk}(\vartheta) \bar{x}_j x_k = \sum_{j,k=1}^{\nu_D} H_{jk}^D \bar{x}_j x_k = \langle H_Dx, x \rangle, \tag{2.29}
\]

\[
\|x\| = \sum_{j=1}^{\nu} |x_j|^2 = \sum_{j=1}^{\nu_D} |x_j|^2. \tag{2.30}
\]

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

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

\[
\lambda_n(\vartheta) \leq \max_{S_{\nu-D-n+1} \subset \mathbb{C}^\nu} \min_{\|x\|=1} \langle H_Dx, x \rangle = \lambda_n^D. \tag{2.32}
\]
Combining (2.26) and (2.32) and using (2.7), we obtain

$$\lambda_n(\vartheta) \in [\lambda_n^N, \lambda_n^D] = J_n, \quad n = 1, \ldots, \nu_D, \quad (2.33)$$

$$\lambda_n(\vartheta) \in [\lambda_n^N, q_n^* + 2\kappa_+] = \tilde{J}_n, \quad n = \nu_D + 1, \ldots, \nu, \quad (2.34)$$

for all $\vartheta \in T_d$.

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

$$\lambda_n(\vartheta) \in [q_n^*, \lambda_n^{N+\nu_N-\nu}] = \tilde{J}_n, \quad n = 1, \ldots, \nu - \nu_D, \quad (2.35)$$

$$\lambda_n(\vartheta) \in [\lambda_n^{D+\nu_D-\nu}, \lambda_n^{N+\nu_N-\nu}] = \tilde{J}_n, \quad n = \nu - \nu_D + 1, \ldots, \nu, \quad (2.36)$$

for all $\vartheta \in T_d$. The relations (2.33) and (2.34) prove (1.20).

**Proof of Theorem 1.2.** i) First, we will prove the estimate (1.23). Let $P$ be the projection onto $\ell^2(\partial V_N)$. Using (1.21) we have

$$\sum_{n=1}^{\nu} |\sigma_n(H)| \leq \sum_{n=1}^{\nu_D} (\lambda_n^D - \lambda_n^N) + \sum_{n=\nu_D+1}^{\nu} (q_n^* + 2\kappa_+ - \lambda_n^N)$$

$$= \text{Tr} H_D - \text{Tr} H_N + \sum_{n=\nu+1}^{\nu_D} \lambda_n^N + \sum_{n=\nu_D+1}^{\nu} (q_n^* + 2\kappa_+)$$

$$= \sum_{n=\nu+1}^{\nu_D} \lambda_n^N + \sum_{n=\nu_D+1}^{\nu} (q_n^* + 2\kappa_+) - \text{Tr}(PH_N).$$

Finally, applying (2.9), (2.10) to the diagonal entries of $PH_N P$, we obtain

$$\sum_{n=1}^{\nu} |\sigma_n(H)| \leq \sum_{n=\nu+1}^{\nu_N} \lambda_n^N + \sum_{n=\nu_D+1}^{\nu} (q_n^* + 2\kappa_+) - \sum_{n=\nu_D+1}^{\nu_N} (\rho_n (\zeta_n^N - \zeta_{nn}^N) + q_n^N)$$

$$= \sum_{n=\nu+1}^{\nu_D} \lambda_n^N + \sum_{n=\nu_D+1}^{\nu} (q_n^* + 2\kappa_+ - \rho_n (\zeta_n - \zeta_{nn} + q_n)). \quad (2.35)$$

Here we have used the following identities

$$\sum_{n=\nu_D+1}^{\nu_N} \rho_n \zeta_n^N = \sum_{n=\nu_D+1}^{\nu} \rho_n \sum_{v \in V_n} \zeta_v^N = \sum_{n=\nu_D+1}^{\nu} \rho_n \zeta_n,$$

$$\sum_{n=\nu_D+1}^{\nu_N} \rho_n \zeta_{nn}^N = \sum_{n=\nu_D+1}^{\nu} \rho_n \zeta_{nn}, \quad \sum_{n=\nu_D+1}^{\nu_N} q_n^N = \sum_{n=\nu_D+1}^{\nu} \rho_n q_n.$$

Thus, the estimate (1.23) has proved.
Second, using (1.21) and (1.22) we have
\[
\sum_{n=1}^\nu |\sigma_n(H)| \leq \sum_{n=1}^{\nu_D} (\lambda_n^N - \lambda_n^v) + \sum_{n=\nu_D+1}^{\nu-\nu_D} (\lambda_n^{N+\nu} - \lambda_n^N)
+ \sum_{n=\nu-\nu_D+1}^\nu (\lambda_n^N - \lambda_n^{N+\nu_D}) = \sum_{n=\nu_D+1}^\nu \lambda_n^{N+\nu_D} - \sum_{n=1}^{\nu-\nu_D} \lambda_n^N
= \sum_{n=1}^{\nu-\nu_D} \lambda_{\nu_N-\nu_D+n} - \sum_{n=1}^{\nu-\nu_D} \lambda_n^N.
\]
Thus, the estimate (1.24) has also proved.

ii) First, we will prove that 0 ≤ ν_D ≤ ν − 1. It is clear that 0 ≤ ν_D and, for example, for the square lattice ν_D = 0. For the graph shown in Fig. 2, ν_D = ν − 1. Assume that ν_D = ν. Then the graph Γ_N contains all bridges of Γ. This contradicts the construction of Γ_N.

Consider the Laplacian ∆ on the periodic graph Γ shown in Fig. 1. For each \( \vartheta \in \mathbb{T}^d \) the matrix \( \Delta(\vartheta) \) defined by (2.5) has the form
\[
\Delta(\vartheta) = \begin{pmatrix}
6 & -\Delta_{12}(\vartheta) & -1 - e^{-i\vartheta_2} \\
-\Delta_{12}(\vartheta) & 4 & 0 \\
-1 - e^{i\vartheta_2} & 0 & 2
\end{pmatrix},
\]
\[
\Delta_{12}(\vartheta) = 1 + e^{i\vartheta_1} + e^{-i\vartheta_2} + e^{i(\vartheta_1-\vartheta_2)}.
\]

The characteristic polynomial of \( \Delta(\vartheta) \) is given by
\[
\det(\Delta(\vartheta) - \lambda \mathbb{1}_3) = -\lambda^3 + 12\lambda^2 + 2 (2c_1c_2 + 2c_1 + 3c_2 - 19)\lambda - 4 (2c_1c_2 + 2c_1 + 4c_2 - 8),
\]
\[
c_1 = \cos \vartheta_1, \quad c_2 = \cos \vartheta_2.
\]

The spectrum of the Laplacian \( \Delta \) on the periodic graph Γ consists of three bands:
\[
\sigma_1 = [0; 2], \quad \sigma_2 \approx [2.5; 4], \quad \sigma_3 \approx [6; 9.5].
\]
The matrices $H_N$ and $H_D$, defined by (2.9) – (2.11), in this case have the form

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

The spectra of the operators $H_N$ and $H_D$ are

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

Thus, the intervals $J_n$ and $\tilde{J}_n$ defined by (1.21), (1.22) and their intersections $J_n \cap \tilde{J}_n$, $n \in \mathbb{N}_3$, have the form

- $J_1 = [0; 6]$, $\tilde{J}_1 = [0, 4]$, $\sigma_1 = [0; 2] \subset J_1 \cap \tilde{J}_1 = J_1 = [0; 4]$;
- $J_2 = [2; 12]$, $\tilde{J}_2 = [0; 4]$, $\sigma_2 \approx [2.5; 4] \subset J_2 \cap \tilde{J}_2 = [2; 4]$;
- $J_3 \approx [2.5; 12]$, $\tilde{J}_3 \approx [6; 9.5]$, $\sigma_3 \approx [6; 9.5] = J_3 \cap \tilde{J}_3 = \tilde{J}_3$.

**Remark.**

1) Theorem 1.1 determines the existence of the second spectral gap (see Fig.1b). 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 $\lambda_n(\vartheta) \leq 2\kappa_+ = 12$ that is trivial. But using (1.20) 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 Fig.1a the estimates (1.23), (1.24) have the form

$$\sum_{n=1}^3 |\sigma_n(H)| \leq \sum_{n=2}^3 (12 - h_n) + \sum_{n=4}^7 \lambda_n^N \approx 4 + 12 + 9.5 = 25.5, \quad (2.38)$$

$$\sum_{n=1}^3 |\sigma_n(H)| \leq \sum_{n=1}^2 (\lambda_{5+n}^N - \lambda_3^N) \approx 9.5 + 4 - 2 = 11.5. \quad (2.39)$$

Thus, the estimate (2.39) is much better than (2.38). Finally, we note that (2.37) yields

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

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