PROCEEDINGS OF THE
AMERICAN MATHEMATICAL SOCIETY
Volume 143, Number 9, September 2015, Pages 3951–3967
S 0002-9939(2015)12586-5
Article electronically published on March 27, 2015

SPECTRAL BAND LOCALIZATION FOR SCHRÖDINGER OPERATORS ON DISCRETE PERIODIC GRAPHS

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(Communicated by Joachim Krieger)

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, $d \geqslant 2$. 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 $\sigma_n = [a_{n-1}^+, a_n^-]$, where

$$a_{n-1}^+ < a_n^- \leqslant a_n^+, \quad n \geqslant 1, \qquad a_n^\pm = (\pi n)^2 + O(1) \quad \text{as } n \to \infty. \tag{1.1}$$

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

$$-f'' + qf = \lambda f, \qquad f(0) = f(1) = 0, \qquad \lambda \in \mathbb{C}, \tag{1.2}$$

where q is the periodic potential restricted on the unit interval. Let $D_n, n \geqslant 1$, be the Dirichlet eigenvalues, that is, the eigenvalues of the problem (1.2).

Received by the editors October 13, 2013 and, in revised form, May 18, 2014.
2010 *Mathematics Subject Classification.* Primary 47A10.
Key words and phrases. Schrödinger operator, periodic discrete graph, spectral band localization.

We also consider the Sturm-Liouville problem on the unit interval with the Neumann boundary conditions:

$$-f'' + qf = \lambda f, \qquad f'(0) = f'(1) = 0, \qquad \lambda \in \mathbb{C}. \tag{1.3}$$

Let $N_n, n \geqslant 1$, be the Neumann eigenvalues, that is, the eigenvalues of the problem (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 $n \geqslant 1$. Thus we obtain

$$\sigma_n \subset [N_n, D_n], \qquad \forall\, n \in \mathbb{N}. \tag{1.4}$$

This is a simple example of Dirichlet-Neumann bracketing. For more complicated examples see [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 [LP08] obtained Dirichlet-Neumann bracketing for the Laplacian on periodic metric graphs. Via an explicit Cattaneo correspondence [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 [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 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 [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 $\Gamma = (V, \mathcal{E})$ be a connected graph, possibly having loops and multiple edges, where V is the set of its vertices and $\mathcal{E}$ is the set of its unoriented edges. An edge connecting vertices u and v from V will be denoted as the unordered pair $(u, v)_e \in \mathcal{E}$ 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 $(u, v)_e \in \mathcal{E}$. For each vertex $v \in V$ we define the degree $\varkappa_v = \deg v$ as the number of all its incident edges from $\mathcal{E}$ (here a loop is counted twice). Below we consider locally finite $\mathbb{Z}^d$-periodic graphs Γ, 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 $a_1, \dots, a_d$ in $\mathbb{R}^d$ (the so-called periods of Γ) such that Γ is invariant under translations through the vectors $a_1, \dots, a_d$:

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

From this definition it follows that a $\mathbb{Z}^d$-periodic graph Γ is invariant under translations through any integer vector (in the basis $a_1, \dots, a_d$):

$$\Gamma + \mathrm{m} = \Gamma, \qquad \forall\, \mathrm{m} \in \mathbb{Z}^d.$$

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

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

We define the self-adjoint Laplacian (or the Laplace operator) Δ on $f \in \ell^2(V)$ by

$$\big(\Delta f\big)(v) = \sum_{(v,\, u)_e \in \mathcal{E}} \big(f(v) - f(u)\big) \qquad \forall\, v \in V. \tag{1.5}$$

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

$$0 \in \sigma(\Delta) \subset [0, 2\varkappa_+], \qquad \text{where} \qquad \varkappa_+ = \sup_{v \in V} \deg v < \infty. \tag{1.6}$$

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

$$H = \Delta + Q, \tag{1.7}$$

$$\big(Qf\big)(v) = Q(v) f(v) \qquad \forall\, v \in V, \tag{1.8}$$

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

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

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

$$\Gamma_F = \Gamma/\mathbb{Z}^d \subset \mathbb{R}^d/\mathbb{Z}^d. \tag{1.9}$$

The fundamental graph Γ_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 $a_1, \dots, a_d$. Below the coordinates of all vertices of Γ 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

$$V_F = [0, 1)^d \cap V = \{v_1, \dots, v_\nu\}, \qquad \nu = \#V_F < \infty, \tag{1.10}$$

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

$$\ell^2(V) = \frac{1}{(2\pi)^d} \int_{\mathbb{T}^d}^{\oplus} \ell^2(V_F)\, d\vartheta, \qquad UHU^{-1} = \frac{1}{(2\pi)^d} \int_{\mathbb{T}^d}^{\oplus} H(\vartheta) d\vartheta, \tag{1.11}$$

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

$$H(\vartheta) = \Delta(\vartheta) + q, \qquad q = \mathrm{diag}(q_1, \dots, q_\nu), \qquad \forall\, \vartheta \in \mathbb{T}^d, \tag{1.12}$$

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

$$Q(v_j) = q_j, \qquad j \in \mathbb{N}_\nu = \{1, \dots, \nu\}. \tag{1.13}$$

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 Δ is given by (2.5). Each Floquet $\nu \times \nu$ matrix $H(\vartheta)$, $\vartheta \in \mathbb{T}^d$, has ν eigenvalues labeled by

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

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

$$\sigma_n(H) = [\lambda_n^-, \lambda_n^+] = \lambda_n(\mathbb{T}^d). \tag{1.14}$$

Thus, the spectrum of the operator H on the periodic graph Γ is given by

$$\sigma(H) = \bigcup_{\vartheta \in \mathbb{T}^d} \sigma\big(H(\vartheta)\big) = \bigcup_{n=1}^{\nu} \sigma_n(H). \tag{1.15}$$

Note that if $\lambda_n(\cdot) = C_n = \text{const}$ on some set $\mathscr{B} \subset \mathbb{T}^d$ of positive Lebesgue measure, then the operator H on Γ 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 Γ has the form

$$\sigma(H) = \sigma_{ac}(H) \cup \sigma_{fb}(H), \tag{1.16}$$

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 Γ is called a *fundamental domain* of Γ 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) Γ_1 *does not contain any* $\mathbb{Z}^d$*-equivalent edges;*

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

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 Γ_1 is not uniquely defined and we fix one of them. Let $\varkappa_v^1$ be the degree of the vertex $v \in V_1$ on Γ_1. A vertex $v \in V_1$ is called an *inner* vertex of Γ_1, if $\varkappa_v = \varkappa_v^1$, i.e., if all its incident edges $\mathbf{e} \in \mathcal{E}$ also belong to $\mathcal{E}_1$. Denote by V_o the set of all inner vertices of Γ_1. We define a *boundary* ∂V_1 of Γ_1 by the standard identity:

$$\partial V_1 = V_1 \setminus V_o. \tag{1.17}$$

Example 1. We consider the square lattice Γ. We choose the periods of the graph a_1, a_2 as shown in Figure 1. A fundamental domain Γ_1, the inner vertices and the boundary are shown in Figure 1. In this simple situation the definitions of V_o and ∂V_1 are quite clear and natural. But for more complicated graphs the situation may be rather difficult (see Figure 3).

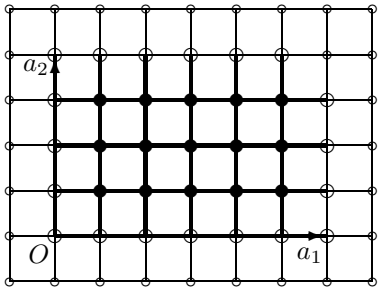

FIGURE 1. The square lattice Γ and its fundamental domain Γ_1; the vertices of the graph Γ_1 are big points (black and white); the edges of Γ_1 are marked by bold lines. The inner vertices are black points, the boundary vertices are white points.

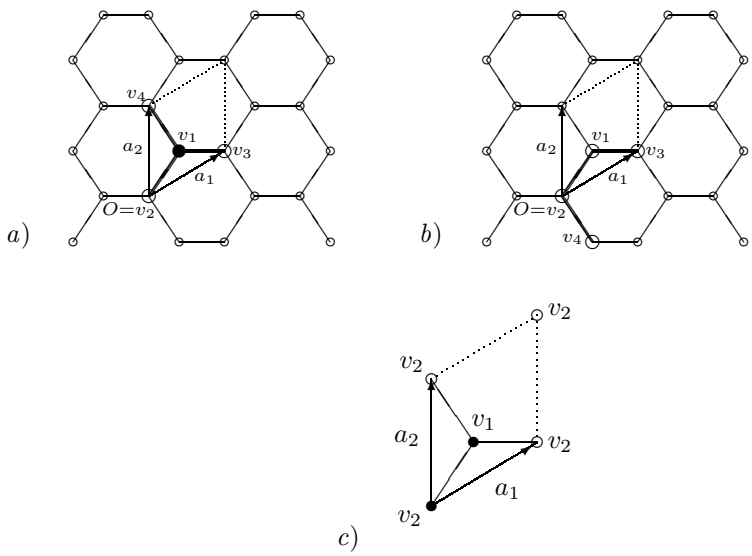

FIGURE 2. *a*) The fundamental domain Γ_1 of the hexagonal lattice; $V_1 = \{v_1, v_2, v_3, v_4\}$, the inner vertex set and the boundary are $V_o = \{v_1\}$, $\partial V_1 = \{v_2, v_3, v_4\}$, respectively. *b*) Another finite graph Γ_1 of the hexagonal lattice; $V_o = \varnothing$, $\partial V_1 = V_1 = \{v_1, v_2, v_3, v_4\}$. *c*) The fundamental graph Γ_F of the hexagonal lattice; the vertices of Γ_F are black.

Example 2. For the hexagonal lattice with periods a_1, a_2 (see Figure 2) we can choose a fundamental domain Γ_1 by two different not isomorphic ways (see Figure 2*a*,*b*). The numbers of the inner vertices and the boundary vertices depend on the choice of the graph Γ_1. The first graph Γ_1 (see Figure 2*a*) has one inner vertex and 3 boundary vertices. But for another graph Γ_1 (see Figure 2*b*) the set of the inner vertices is empty and $V_1 = \partial V_1$.

Remark. 1) If the graph Γ_1 is "rather big", then the number of the inner vertices is significantly greater than the number of the boundary vertices. If the graph Γ_1

is "rather small", then the set V_o may be empty and all vertices of Γ_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 2.1).

On the finite graph Γ_1 we define two self-adjoint operators H_1 and H_o:

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

$$H_1 = \Delta_1 + Q, \qquad \Delta_1 = \sqrt{\rho}\Delta_* \sqrt{\rho}\,, \tag{1.18}$$

where Δ_* is the Laplacian on the graph Γ_1, defined by (1.5). Furthermore, $\sqrt{\rho} > 0$, and $\rho > 0$ is the multiplication operator on $\ell^2(V_1)$ given by

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

i.e., ρ_v is the number of vertices from V_1 equivalent to v with respect to the actions of the group $\mathbb{Z}^d$, $1 \leqslant \rho_v \leqslant \nu_1$, 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_o on $f \in \ell^2(V_1)$ is defined by

$$H_o f = H_1 f, \quad \text{where} \quad f|_{\partial V_1} = 0. \tag{1.20}$$

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

Remark. 1) The operator Δ_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_o the Dirichlet operator.

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

$$\lambda_1^\phi \leqslant \lambda_2^\phi \leqslant \ldots \leqslant \lambda_{\nu_\phi}^\phi, \qquad \nu_\phi = \#V_\phi, \quad \phi = o, 1. \tag{1.21}$$

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

$$q_1^\bullet \leqslant q_2^\bullet \leqslant \ldots \leqslant q_\nu^\bullet. \tag{1.22}$$

Here $q_1^\bullet = q_{n_1}, q_2^\bullet = q_{n_2}, \ldots, q_\nu^\bullet = q_{n_\nu}$ 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 Γ satisfies*

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

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

$$J_n = \begin{cases} [\lambda_n^1, \lambda_n^o], & n = 1, \ldots, \nu_o, \\ [\lambda_n^1, q_n^\bullet + 2\varkappa_+], & n = \nu_o + 1, \ldots, \nu, \end{cases} \tag{1.24}$$

and

$$\widetilde{J}_n = \begin{cases} [q_n^\bullet, \lambda_{n+\nu_1-\nu}^1], & n = 1, \ldots, \nu - \nu_o, \\ [\lambda_{n-\nu+\nu_o}^o, \lambda_{n+\nu_1-\nu}^1], & n = \nu - \nu_o + 1, \ldots, \nu. \end{cases} \tag{1.25}$$

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 $\hat{\Delta} = \varkappa^{-1/2}\Delta\varkappa^{-1/2}$, where $\varkappa^{1/2} > 0$ and $\varkappa > 0$ is the multiplication operator on $\ell^2(V)$ given by

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

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

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

3) Theorem 1.1 estimates the positions of the spectral bands in terms of eigenvalues of the operators H_1 and H_o on a fundamental domain Γ_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*a* in the case when $H = \Delta$ the intervals $J_n \cap \widetilde{J}_n$, $n \in \mathbb{N}_3$, are shown in Figure 3*c*. The spectrum of the Laplacian Δ 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).

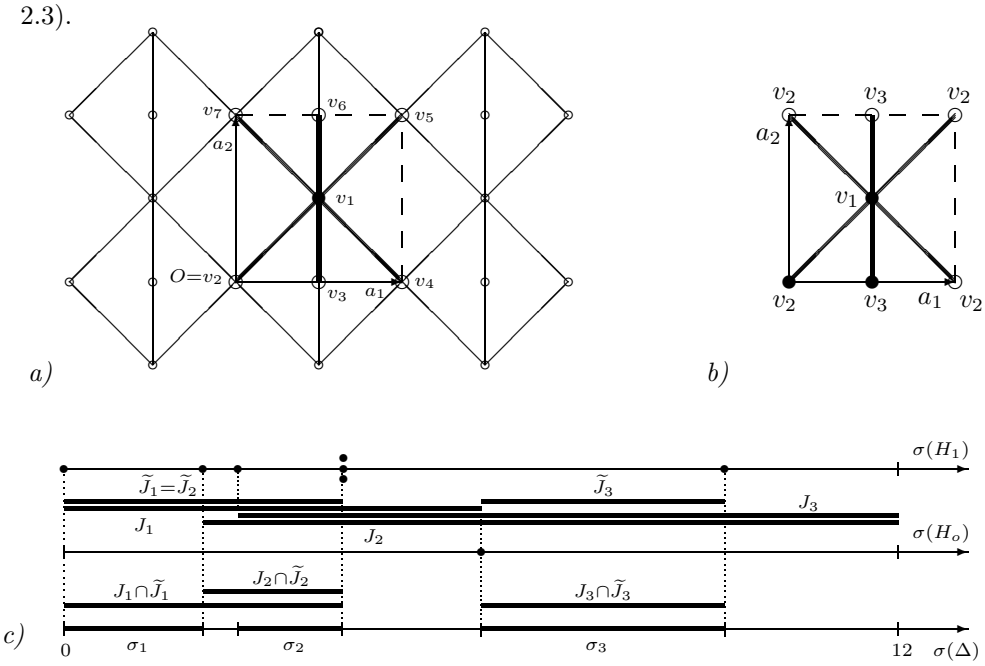

FIGURE 3. *a)* A periodic graph Γ and its fundamental domain Γ_1, the vertices of Γ_1 are big points (white and black); the edges of Γ_1 are marked by bold lines. The set of the inner vertices (black points) and the boundary (white points) are $V_o = \{v_1\}$ and $\partial V_1 = \{v_2, v_3, v_4, v_5, v_6, v_7\}$, respectively. *b)* The fundamental graph Γ_F; the vertices of Γ_F are black. *c)* Eigenvalues of the operators H_1 and H_o, the intervals J_n and $\widetilde{J}_n$, $n \in \mathbb{N}_3$, and their intersections, the spectrum of the Laplacian Δ.

4) Generally speaking, for distinct fundamental domains Γ_1 the operators H_1, H_o, their eigenvalues and, consequently, the intervals $J_n, \widetilde{J}_n$ are different. We number

the fundamental domains $\Gamma_1^1, \Gamma_1^2, \dots$. Thus, a more precise localization of the spectral bands of the Schrödinger operators H on a periodic graph Γ has the form

$$\sigma_n(H) \subset \bigcap_\alpha \big(J_n^\alpha \cap \widetilde{J}_n^\alpha\big), \qquad n \in \mathbb{N}_\nu, \tag{1.26}$$

where $J_n^\alpha, \widetilde{J}_n^\alpha$ are the intervals, defined by (1.24), (1.25), for the fundamental domain Γ_1^α. 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*

$$\sum_{n=1}^{\nu} |\sigma_n(H)| \leqslant \sum_{n=\nu_o+1}^{\nu} (q_n^\bullet + 2\varkappa_+ - h_n) + \sum_{n=\nu+1}^{\nu_1} \lambda_n^1, \tag{1.27}$$
$$\text{where} \quad h_n = \rho_n(\varkappa_n - \varkappa_{nn} + q_n), \qquad \rho_n = \#\mathcal{Z}(v_n),$$

$\varkappa_{nn}$ is the number of loops of the vertex v_n on the graph Γ;

$$\sum_{n=1}^{\nu} |\sigma_n(H)| \leqslant \sum_{n=1}^{\nu-\nu_o} \big(\lambda^1_{\nu_1-(\nu-\nu_o)+n} - \lambda_n^1\big). \tag{1.28}$$

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

$$0 \leqslant \nu_o \leqslant \nu - 1, \qquad \nu + d \leqslant \nu_1 \leqslant \#\mathcal{E}_F + 1. \tag{1.29}$$

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 $(u, v)_e \in \mathcal{E}$: 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 Γ and the fundamental graph Γ_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:

$$v = [v] + \tilde{v}, \qquad [v] \in \mathbb{Z}^d, \qquad \tilde{v} \in V_F \subset [0, 1)^d. \tag{2.1}$$

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

$$\tau(\mathbf{e}) = [v] - [u] \in \mathbb{Z}^d, \tag{2.2}$$

where due to (2.1) we have

$$u = [u] + \tilde{u}, \qquad v = [v] + \tilde{v}, \qquad [u], [v] \in \mathbb{Z}^d, \qquad \tilde{u}, \tilde{v} \in V_F.$$

If $\mathbf{e} = (u, v)$ is an oriented edge of the graph Γ, then by the definition of the fundamental graph there is an oriented edge $\tilde{\mathbf{e}} = (\tilde{u}, \tilde{v})$ on Γ_F. For the edge $\tilde{\mathbf{e}} \in \mathcal{A}_F$ we define the edge index $\tau(\tilde{\mathbf{e}})$ by

$$\tau(\tilde{\mathbf{e}}) = \tau(\mathbf{e}). \tag{2.3}$$

In other words, edge indices of the fundamental graph Γ_F are induced by edge indices of the periodic graph Γ. 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 Γ. But in a fixed coordinate system the index of the fundamental graph edge is uniquely determined by (2.3), since

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

Edges with non-zero indices will be called *bridges*. For example, for the graph shown in Figure 3*a* 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 (1.11), where the Floquet $\nu \times \nu$ matrix $H(\vartheta)$ has the form

$$H(\vartheta) = \Delta(\vartheta) + q, \qquad q = \mathrm{diag}(q_1, \ldots, q_\nu), \qquad \forall\, \vartheta \in \mathbb{T}^d. \tag{2.4}$$

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

$$\Delta_{jk}(\vartheta) = \varkappa_j \delta_{jk} - \begin{cases} \displaystyle\sum_{\mathbf{e}=(v_j,\, v_k)\in\mathcal{A}_F} e^{\,i\langle \tau(\mathbf{e}),\, \vartheta\rangle}, & \text{if } \ (v_j, v_k) \in \mathcal{A}_F, \\ 0, & \text{if } \ (v_j, v_k) \notin \mathcal{A}_F; \end{cases} \tag{2.5}$$

see [KS13], where $\varkappa_j$ is the degree of v_j, δ_{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 $\lambda_1(A) \leqslant \ldots \leqslant \lambda_\nu(A)$, $\lambda_1(B) \leqslant \ldots \leqslant \lambda_\nu(B)$ the eigenvalues of A and B, respectively, arranged in increasing order, counting multiplicities. Then we have*

$$\lambda_n(A) + \lambda_1(B) \leqslant \lambda_n(A + B) \leqslant \lambda_n(A) + \lambda_\nu(B), \qquad \forall\, n \in \mathbb{N}_\nu. \tag{2.6}$$

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

$$\begin{aligned} &q_n^\bullet \leqslant \lambda_n(\vartheta) \leqslant q_n^\bullet + 2\varkappa_+, \qquad \forall\, (\vartheta, n) \in \mathbb{T}^d \times \mathbb{N}_\nu, \\ &\sigma_n(H) = \lambda_n(\mathbb{T}^d) \subset [q_n^\bullet, q_n^\bullet + 2\varkappa_+], \qquad \forall\, n \in \mathbb{N}_\nu. \end{aligned} \tag{2.7}$$

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 $v = u - \mathrm{m} \in V_F \subset V_1$ for some $0 \neq \mathrm{m} \in \mathbb{Z}^d$. First, we will show that u and v are not adjacent on Γ. Indeed, if $(u, v)_e \in \mathcal{E}$, then, due to the periodicity of Γ, $(u + \mathrm{m}, u)_e \in \mathcal{E}$. Since $u \in V_o$, the incident to u edges $(u, v)_e, (u + \mathrm{m}, u)_e \in \mathcal{E}_1$. Thus, $\mathcal{E}_1$ contains $\mathbb{Z}^d$-equivalent edges, which contradicts the definition of the fundamental domain Γ_1 and we obtain that u and v are not adjacent on Γ ($u \nsim v$). Second, we will

show that $\varkappa_v^1 = 0$, that will contradict the connectivity of Γ_1 and complete the proof. Indeed, since $u \in V_o$, all edges incident to u on Γ are contained in $\mathcal{E}_1$. 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 Γ_1 and the fact that $u \nsim v$, we conclude that $\mathcal{E}_1$ does not contain any edges incident to v. Thus, $\varkappa_v^1 = 0$. □

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 $\Gamma_1 = (V_1, \mathcal{E}_1)$ has the form

$$V_o = \{v_1, \dots, v_{\nu_o}\}.$$

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

$$\mathcal{Z}_j \equiv \mathcal{Z}(v_j) = \big(\{v_j\} + \mathbb{Z}^d\big) \cap V_1, \qquad j \in \mathbb{N}_\nu. \tag{2.8}$$

The Neumann operator H_1 on the graph Γ_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

$$H_1 = \Delta_1 + q^1, \qquad q^1 = \operatorname{diag}(q^1_1, \dots, q^1_{\nu_1}), \tag{2.9}$$

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

$$\Delta^1_{jk} = \sqrt{\rho_j \rho_k}\,\big(\varkappa^1_j \delta_{jk} - \varkappa^1_{jk}\big). \tag{2.10}$$

Here $\varkappa^1_j$ is the degree of the vertex $v_j \in V_1$ on the graph Γ_1, $\varkappa^1_{jk} \geqslant 1$ is the multiplicity of the edge $(v_j, v_k) \in \mathcal{E}_1$ and $\varkappa^1_{jk} = 0$ if $(v_j, v_k) \notin \mathcal{E}_1$, $\rho_j = \rho_{v_j}$ (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

$$H^o_{jk} = H^1_{jk} \qquad \text{for all} \qquad j, k \in \mathbb{N}_{\nu_o}. \tag{2.11}$$

Recall that

$$\varkappa^1_j = \varkappa_j \ \text{ and } \ \rho_j = 1 \ \text{ for all } \ j \in \mathbb{N}_{\nu_o}. \tag{2.12}$$

Proof of Theorem 1.1. We recall well-known facts.

Denote by $\lambda_1(A) \leqslant \ldots \leqslant \lambda_\nu(A)$ the eigenvalues of a self-adjoint $\nu \times \nu$ matrix A, arranged in increasing order, counting multiplicities. Each λ_n satisfies the minimax principle:

$$\lambda_n(A) = \min_{S_n \subset \mathbb{C}^\nu} \max_{\substack{\|x\|=1 \\ x \in S_n}} \langle Ax, x\rangle, \tag{2.13}$$

$$\lambda_n(A) = \max_{S_{\nu-n+1} \subset \mathbb{C}^\nu} \min_{\substack{\|x\|=1 \\ x \in S_{\nu-n+1}}} \langle Ax, x\rangle, \tag{2.14}$$

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 ν-dimensional subspace Y_ϑ of $\mathbb{C}^{\nu_1}$ by

$$Y_\vartheta = \big\{x = (x_k)_{k=1}^{\nu_1} \in \mathbb{C}^{\nu_1} : \forall\, k = \nu+1, \dots, \nu_1 \quad x_k = e^{\,i\langle v_k - v_j,\, \vartheta\rangle}\, x_j\,, \\ \text{where } j = j(k) \in \mathbb{N}_\nu \text{ is such that } v_k \in \mathcal{Z}_j\big\}. \tag{2.15}$$

Note that $j = j(k)$ in (2.15) is uniquely defined for each $k = \nu+1, \dots, \nu_1$. Let $1 \leqslant n \leqslant \nu$. Using (2.13) and (2.14) we write

$$\lambda_j^1 = \min_{S_j \subset \mathbb{C}^{\nu_1}} \max_{\substack{\|x\|=1 \\ x \in S_j}} \langle H_1 x, x\rangle \geqslant \min_{S_j \subset \mathbb{C}^{\nu_1}} \max_{\substack{\|x\|=1 \\ x \in S_j \cap Y_\vartheta}} \langle H_1 x, x\rangle, \quad j = n + \nu_1 - \nu, \tag{2.16}$$

$$\lambda_n^1 = \max_{S_k \subset \mathbb{C}^{\nu_1}} \min_{\substack{\|x\|=1 \\ x \in S_k}} \langle H_1 x, x\rangle \leqslant \max_{S_k \subset \mathbb{C}^{\nu_1}} \min_{\substack{\|x\|=1 \\ x \in S_k \cap Y_\vartheta}} \langle H_1 x, x\rangle, \quad k = \nu_1 - n + 1, \tag{2.17}$$

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

$$\langle H_1 x, x\rangle = \sum_{j,k=1}^{\nu_1} H_{jk}^1 \, \bar{x}_j \, x_k = \sum_{j=1}^{\nu_1} (\rho_j \varkappa_j^1 + q_j^1)|x_j|^2 - \sum_{j,k=1}^{\nu_1} \varkappa_{jk}^1 \sqrt{\rho_j \rho_k} \, \bar{x}_j \, x_k, \tag{2.18}$$

where

$$\begin{aligned} \sum_{j=1}^{\nu_1} (\rho_j \varkappa_j^1 + q_j^1)|x_j|^2 &= \sum_{j=1}^{\nu_o} (\varkappa_j + q_j)|x_j|^2 + \sum_{j=\nu_o+1}^{\nu} |x_j|^2 \sum_{v \in \mathcal{Z}_j} (\rho_j \varkappa_v^1 + q_j) \\ &= \sum_{j=1}^{\nu_o} (\varkappa_j + q_j)|x_j|^2 + \sum_{j=\nu_o+1}^{\nu} \rho_j (\varkappa_j + q_j)|x_j|^2, \end{aligned} \tag{2.19}$$

$$\sum_{j,k=1}^{\nu_1} \varkappa_{jk}^1 \sqrt{\rho_j \rho_k} \, \bar{x}_j \, x_k = \sum_{j,k=1}^{\nu} \sqrt{\rho_j \rho_k} \sum_{\mathbf{e}=(v_j, v_k) \in \mathcal{A}_F} e^{i\langle \tau(\mathbf{e}), \vartheta\rangle} \, \bar{x}_j \, x_k. \tag{2.20}$$

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

$$\sum_{v \in \mathcal{Z}_j} \varkappa_v^1 = \varkappa_j. \tag{2.21}$$

We introduce the new vector

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

Since $\rho_j = 1$ for $1 \leqslant j \leqslant \nu_o$, we have $y_j = x_j$, $j \in \mathbb{N}_{\nu_o}$ and for $x \in Y_\vartheta$ we obtain

$$\|x\|^2 = \sum_{j=1}^{\nu_1} |x_j|^2 = \sum_{j=1}^{\nu_o} |x_j|^2 + \sum_{j=\nu_o+1}^{\nu} \rho_j \, |x_j|^2 = \sum_{j=1}^{\nu} |y_j|^2 = \|y\|^2. \tag{2.23}$$

Combining (2.18) – (2.20) for $x \in Y_\vartheta$, (2.22) and the definition of $H(\vartheta)$ in (2.4) we obtain

$$\langle H_1 x, x\rangle = \sum_{j=1}^{\nu} (\varkappa_j + q_j)|y_j|^2 - \sum_{j,k=1}^{\nu} \sum_{\mathbf{e}=(v_j, v_k) \in \mathcal{A}_F} e^{i\langle \tau(\mathbf{e}), \vartheta\rangle} \, \bar{y}_j \, y_k = \langle H(\vartheta) y, y\rangle. \tag{2.24}$$

This, (2.16), (2.17), (2.23) and the minimax principle (2.13), (2.14) yield for $1 \leqslant n \leqslant \nu$:

$$\lambda_{n+\nu_1-\nu}^1 \geqslant \min_{S_n \subset \mathbb{C}^\nu} \max_{\substack{\|y\|=1 \\ y \in S_n}} \langle H(\vartheta) y, y\rangle = \lambda_n(\vartheta)\,, \tag{2.25}$$

$$\lambda_n^1 \leqslant \max_{S_{\nu-n+1} \subset \mathbb{C}^\nu} \min_{\substack{\|y\|=1 \\ y \in S_{\nu-n+1}}} \langle H(\vartheta) y, y\rangle = \lambda_n(\vartheta)\,. \tag{2.26}$$

Second, let $X = \{x \in \mathbb{C}^\nu : x_{\nu_o+1} = \ldots = x_\nu = 0\}$ be the ν_o-dimensional subspace of $\mathbb{C}^\nu$ and let $1 \leqslant n \leqslant \nu_o$. Using (2.13) and (2.14) we write

$$\lambda_j(\vartheta) = \min_{S_j \subset \mathbb{C}^\nu} \max_{\substack{\|x\|=1 \\ x \in S_j}} \langle H(\vartheta)x, x\rangle \geqslant \min_{S_j \subset \mathbb{C}^\nu} \max_{\substack{\|x\|=1 \\ x \in S_j \cap X}} \langle H(\vartheta)x, x\rangle, \quad j = n+\nu-\nu_o\,, \tag{2.27}$$

$$\lambda_n(\vartheta) = \max_{S_k \subset \mathbb{C}^\nu} \min_{\substack{\|x\|=1 \\ x \in S_k}} \langle H(\vartheta)x, x\rangle \leqslant \max_{S_k \subset \mathbb{C}^\nu} \min_{\substack{\|x\|=1 \\ x \in S_k \cap X}} \langle H(\vartheta)x, x\rangle, \quad k = \nu-n+1. \tag{2.28}$$

For $x \in X$ we have

$$\langle H(\vartheta)x, x\rangle = \sum_{j,k=1}^{\nu} H_{jk}(\vartheta)\, \bar{x}_j\, x_k = \sum_{j,k=1}^{\nu_o} H^o_{jk}\, \bar{x}_j\, x_k = \langle H_o x, x\rangle, \tag{2.29}$$

$$\|x\| = \sum_{j=1}^{\nu} |x_j|^2 = \sum_{j=1}^{\nu_o} |x_j|^2. \tag{2.30}$$

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

$$\lambda_{n+\nu-\nu_o}(\vartheta) \geqslant \min_{S_n \subset \mathbb{C}^{\nu_o}} \max_{\substack{\|x\|=1 \\ x \in S_n}} \langle H_o x, x\rangle = \lambda^o_n, \tag{2.31}$$

$$\lambda_n(\vartheta) \leqslant \max_{S_{\nu_o-n+1} \subset \mathbb{C}^{\nu_o}} \min_{\substack{\|x\|=1 \\ x \in S_{\nu_o-n+1}}} \langle H_o x, x\rangle = \lambda^o_n. \tag{2.32}$$

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

$$\begin{aligned} &\lambda_n(\vartheta) \in [\lambda^1_n, \lambda^o_n] = J_n, && n = 1, \ldots, \nu_o\,, \\ &\lambda_n(\vartheta) \in [\lambda^1_n, q^\bullet_n + 2\varkappa_+] = J_n, && n = \nu_o+1, \ldots, \nu. \end{aligned} \tag{2.33}$$

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

$$\begin{aligned} &\lambda_n(\vartheta) \in [q^\bullet_n, \lambda^1_{n+\nu_1-\nu}] = \widetilde{J}_n, && n = 1, \ldots, \nu-\nu_o\,, \\ &\lambda_n(\vartheta) \in [\lambda^o_{n+\nu_o-\nu}, \lambda^1_{n+\nu_1-\nu}] = \widetilde{J}_n, && n = \nu-\nu_o+1, \ldots, \nu, \end{aligned} \tag{2.34}$$

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

Proof of Theorem 1.2. i) First, we will prove the estimate (1.27). Let P be the projection onto $\ell^2(\partial V_1)$. Using (1.24) we have

$$\sum_{n=1}^{\nu} |\sigma_n(H)| \leqslant \sum_{n=1}^{\nu_o} (\lambda^o_n - \lambda^1_n) + \sum_{n=\nu_o+1}^{\nu} (q^\bullet_n + 2\varkappa_+ - \lambda^1_n) = \operatorname{Tr} H_o - \operatorname{Tr} H_1$$
$$+ \sum_{n=\nu+1}^{\nu_1} \lambda^1_n + \sum_{n=\nu_o+1}^{\nu} (q^\bullet_n + 2\varkappa_+) = \sum_{n=\nu+1}^{\nu_1} \lambda^1_n + \sum_{n=\nu_o+1}^{\nu} (q^\bullet_n + 2\varkappa_+) - \operatorname{Tr}(PH_1).$$

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

$$\begin{aligned} \sum_{n=1}^{\nu} |\sigma_n(H)| &\leqslant \sum_{n=\nu+1}^{\nu_1} \lambda^1_n + \sum_{n=\nu_o+1}^{\nu} (q^\bullet_n + 2\varkappa_+) - \sum_{n=\nu_o+1}^{\nu_1} \big(\rho_n\,(\varkappa^1_n - \varkappa^1_{nn}) + q^1_n\big) \\ &= \sum_{n=\nu+1}^{\nu_1} \lambda^1_n + \sum_{n=\nu_o+1}^{\nu} \big(q^\bullet_n + 2\varkappa_+ - \rho_n\,(\varkappa_n - \varkappa_{nn} + q_n)\big). \end{aligned} \tag{2.35}$$

Here we have used the following identities:

$$\sum_{n=\nu_o+1}^{\nu_1} \rho_n \varkappa_n^1 = \sum_{n=\nu_o+1}^{\nu} \rho_n \sum_{v\in\mathcal{Z}_n} \varkappa_v^1 = \sum_{n=\nu_o+1}^{\nu} \rho_n \varkappa_n,$$

$$\sum_{n=\nu_o+1}^{\nu_1} \rho_n \varkappa_{nn}^1 = \sum_{n=\nu_o+1}^{\nu} \rho_n \varkappa_{nn}, \qquad \sum_{n=\nu_o+1}^{\nu_1} q_n^1 = \sum_{n=\nu_o+1}^{\nu} \rho_n q_n.$$

Thus, the estimate (1.27) is proved.

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

$$\sum_{n=1}^{\nu} |\sigma_n(H)| \leqslant \sum_{n=1}^{\nu_o} (\lambda_n^o - \lambda_n^1) + \sum_{n=\nu_o+1}^{\nu-\nu_o} (\lambda_{n+\nu_1-\nu}^1 - \lambda_n^1) + \sum_{n=\nu-\nu_o+1}^{\nu} (\lambda_{n+\nu_1-\nu}^1 - \lambda_{n-\nu+\nu_o}^o)$$
$$= \sum_{n=\nu_o+1}^{\nu} \lambda_{n+\nu_1-\nu}^1 - \sum_{n=1}^{\nu-\nu_o} \lambda_n^1 = \sum_{n=1}^{\nu-\nu_o} \lambda_{\nu_1-(\nu-\nu_o)+n} - \sum_{n=1}^{\nu-\nu_o} \lambda_n^1.$$

Thus, the estimate (1.28) is also proved.

ii) First, we will prove that $0 \leqslant \nu_o \leqslant \nu - 1$. We have $0 \leqslant \nu_o$ and $\nu_o = 0$ for some graphs (see, for example, Figure 2*b*). Due to Lemma 2.1, $V_o \subset V_F$ and $\nu_o \leqslant \nu$. Assume that $\nu_o = \nu$, i.e., $V_o = V_F$. Then $\sum_{v\in V_o} \varkappa_v^1 = \sum_{v\in V_o} \varkappa_v = \sum_{v\in V_F} \varkappa_v$. Using this and the fact that $\partial V_1 = V_1 \setminus V_o \neq \varnothing$ we obtain

$$\#\mathcal{E}_1 = \tfrac{1}{2} \sum_{v\in V_1} \varkappa_v^1 > \tfrac{1}{2} \sum_{v\in V_o} \varkappa_v^1 = \tfrac{1}{2} \sum_{v\in V_F} \varkappa_v = \#\mathcal{E}_F.$$

Thus, $\#\mathcal{E}_1 > \#\mathcal{E}_F$. From this we conclude that Γ_1 contains $\mathbb{Z}^d$-equivalent edges, which yields a contradiction. Therefore, $\nu_o \leqslant \nu - 1$ and $\nu_o = \nu - 1$ for some graphs (see Figure 4*a*).

Second, we will show that $\nu + d \leqslant \nu_1 \leqslant \#\mathcal{E}_F + 1$. The connectivity of Γ_1 implies $\nu_1 = \#V_1 \leqslant \#\mathcal{E}_1 + 1$. The definition of the fundamental domain Γ_1 gives that $\#\mathcal{E}_1 = \#\mathcal{E}_F$. Thus, $\nu_1 \leqslant \#\mathcal{E}_F + 1$. Since $\mathbb{Z}^d$-periodic graph Γ is connected, the fundamental domain Γ_1 has at least d bridges. Therefore, $\#(V_1 \setminus V_F) \geqslant d$. This and $V_F \subset V_1$ yield $\nu_1 \geqslant \nu + d$. The example in Figure 2*a* shows that $\nu + d = \nu_1 = \#\mathcal{E}_F + 1$. □

2.3. **Example 3.** Consider the Laplacian $H = \Delta$ on the periodic graph Γ shown in Figure 3*a*. 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 (2.5) has the form

(2.36)
$$\Delta(\vartheta) = \begin{pmatrix} 6 & -\Delta_{12}(\vartheta) & -1 - e^{i\vartheta_2} \\ -\bar{\Delta}_{12}(\vartheta) & 4 & 0 \\ -1 - e^{-i\vartheta_2} & 0 & 2 \end{pmatrix}, \quad \Delta_{12}(\vartheta) = (1 + e^{i\vartheta_1})(1 + e^{i\vartheta_2}).$$

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

$$\det(\Delta(\vartheta) - \lambda \mathbb{1}_3) = -\lambda^3 + 12\lambda^2 + 2\,(2c_1c_2 + 2c_1 + 3c_2 - 19)\lambda - 4(2c_1c_2 + 2c_1 + 4c_2 - 8),$$

$\mathbb{1}_3$ is the 3×3 identity matrix, $c_1 = \cos\vartheta_1$, $c_2 = \cos\vartheta_2$. The spectrum of the Laplacian Δ on the periodic graph Γ consists of three bands:

$$\sigma_1 = [0; 2], \qquad \sigma_2 \approx [2.5; 4], \qquad \sigma_3 \approx [6; 9.5]. \tag{2.37}$$

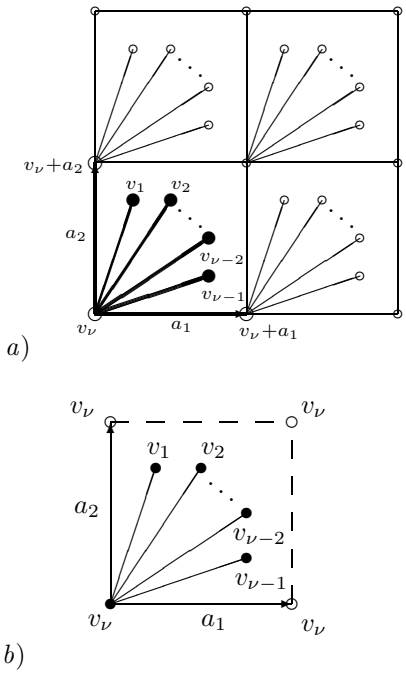

FIGURE 4. *a*) $\mathbb{Z}^2$-periodic graph and its fundamental domain (in bold) with $\nu_o = \nu - 1$. *b*) The fundamental graph Γ_F; the vertices of Γ_F are black.

The fundamental domain $\Gamma_1 = (V_1, \mathcal{E}_1)$ shown in Figure 3*a* 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 ∂V_1 of Γ_1 have the form

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

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

$$H_1 = \begin{pmatrix} 6 & A \\ A^T & D \end{pmatrix}, \quad A = -\begin{pmatrix} 2 & \sqrt{2} & 2 & 2 & \sqrt{2} & 2 \end{pmatrix},$$
$$D = \mathrm{diag}(4, 2, 4, 4, 2, 4), \quad H_o = 6.$$

The spectra of the operators H_1 and H_o are

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

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

$$\begin{array}{lll} J_1 = [0; 6], & \widetilde{J}_1 = [0, 4], & \sigma_1 = [0; 2] \subset J_1 \cap \widetilde{J}_1 = J_1 = [0; 4], \\ J_2 = [2; 12], & \widetilde{J}_2 = [0; 4], & \sigma_2 \approx [2.5; 4] \subset J_2 \cap \widetilde{J}_2 = [2; 4], \\ J_3 \approx [2.5; 12], & \widetilde{J}_3 \approx [6; 9.5], & \sigma_3 \approx [6; 9.5] = J_3 \cap \widetilde{J}_3 = \widetilde{J}_3. \end{array} \tag{2.38}$$

Remark. 1) Theorem 1.1 determines the existence of the second spectral gap (see Figure 3*c*). The intersection of the intervals J_n and $\widetilde{J}_n$, $n = 1, 2, 3$, 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 $\lambda_n(\vartheta) \leqslant 2\varkappa_+ = 12$ 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*a* the estimates (1.27), (1.28) have the form

$$\sum_{n=1}^{3} |\sigma_n(H)| \leqslant \sum_{n=2}^{3} (12 - h_n) + \sum_{n=4}^{7} \lambda_n^1 \approx 25.5, \quad \sum_{n=1}^{3} |\sigma_n(H)| \leqslant \sum_{n=1}^{2} \left(\lambda_{5+n}^1 - \lambda_n^1\right) \approx 11.5.$$

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

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

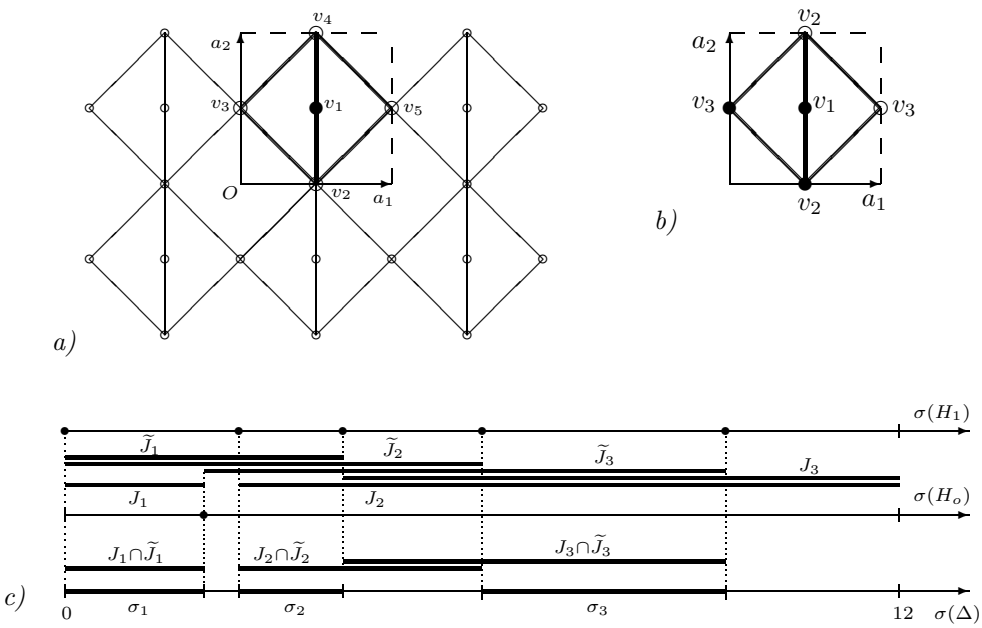

FIGURE 5. *a)* The same periodic graph Γ and another fundamental domain Γ_1. The set of the inner vertices (black points) and the boundary (white points) are $V_o = \{v_1\}$ and $\partial V_1 = \{v_2, v_3, v_4, v_5\}$, respectively. *b)* The fundamental graph Γ_F; the vertices of Γ_F are black. *c)* Eigenvalues of the operators H_1 and H_o, the intervals J_n and $\widetilde{J}_n$, $n \in \mathbb{N}_3$, and their intersections, the spectrum of the Laplacian Δ.

Example 4. We can choose the fundamental graph Γ_1 for the periodic graph Γ in Example 3 by another way as shown in Figure 5*a*. 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

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

The spectra of the operators H_1 and H_o are

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

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

$$\begin{array}{lll} J_1 = [0;2], & \widetilde{J}_1 = [0,4], & \sigma_1 = [0;2] = J_1 \cap \widetilde{J}_1 = J_1, \\ J_2 \approx [2.5;12], & \widetilde{J}_2 = [0;6], & \sigma_2 \approx [2.5;4] \subset J_2 \cap \widetilde{J}_2 \approx [2.5;6], \\ J_3 = [4;12], & \widetilde{J}_3 \approx [2;9.5], & \sigma_3 \approx [6;9.5] \subset J_3 \cap \widetilde{J}_3 \approx [4;9.5]. \end{array} \tag{2.39}$$

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

$$\begin{aligned} \sigma_1 &= [0;2] \subset [0;4] \cap [0;2] = [0;2], \\ \sigma_2 &\approx [2.5;4] \subset [2;4] \cap [2.5;6] = [2.5;4], \\ \sigma_3 &\approx [6;9.5] \subset [6;9.5] \cap [4;9.5] = [6;9.5]. \end{aligned}$$

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

$$\sum_{n=1}^{3} |\sigma_n(H)| \leqslant \sum_{n=2}^{3} (12 - h_n) + \sum_{n=4}^{5} \lambda_n^1 \approx 19.5, \qquad \sum_{n=1}^{3} |\sigma_n(H)| \leqslant \sum_{n=1}^{2} \left(\lambda_{3+n}^1 - \lambda_n^1\right) \approx 13.$$

Acknowledgements

Various parts of this paper were written during the first author's stay at the Centre for Quantum Geometry of Moduli Spaces (QGM), Aarhus University, Denmark. He is grateful to the institute for the hospitality. His study was partly supported by the RFFI grant "Spectral and asymptotic methods for studying of the differential operators" No 11-01-00458 and by the project SPbGU No 11.38.215.2014.

References

[C97] Carla Cattaneo, *The spectrum of the continuous Laplacian on a graph*, Monatsh. Math. **124** (1997), no. 3, 215–235, DOI 10.1007/BF01298245. MR1476363 (98j:35127)

[HJ85] Roger A. Horn and Charles R. Johnson, *Matrix analysis*, Cambridge University Press, Cambridge, 1985. MR832183 (87e:15001)

[K98] Evgeni Korotyaev, *Estimates of periodic potentials in terms of gap lengths*, Comm. Math. Phys. **197** (1998), no. 3, 521–526, DOI 10.1007/s002200050462. MR1652779 (99h:34125)

[K03] Evgeni Korotyaev, *Characterization of the spectrum of Schrödinger operators with periodic distributions*, Int. Math. Res. Not. **37** (2003), 2019–2031, DOI 10.1155/S1073792803209107. MR1995145 (2004e:34134)

[KS13] E. Korotyaev and N. Saburova, *Schrödinger operators on periodic discrete graphs*, Journal of Mathematical Analysis and Applications, 420.1 (2014), 576-611.

[LS75] B. M. Levitan and I. S. Sargsyan, *Introduction to spectral theory*, Translations of Mathematical Monographs. Amer. Math. Soc., Vol. 39, 1975.

[LP08] Fernando Lledó and Olaf Post, *Eigenvalue bracketing for discrete and metric graphs*, J. Math. Anal. Appl. **348** (2008), no. 2, 806–833, DOI 10.1016/j.jmaa.2008.07.029. MR2446037 (2010a:47076)

[Me94] Russell Merris, *Laplacian matrices of graphs: a survey*, Linear Algebra Appl. **197/198** (1994), 143–176, DOI 10.1016/0024-3795(94)90486-3. Second Conference of the International Linear Algebra Society (ILAS) (Lisbon, 1992). MR1275613 (95e:05084)

[M92] Bojan Mohar, *Laplace eigenvalues of graphs—a survey*, Discrete Math. **109** (1992), no. 1-3, 171–183, DOI 10.1016/0012-365X(92)90288-Q. Algebraic graph theory (Leibnitz, 1989). MR1192380 (93m:05133)

[MW89] Bojan Mohar and Wolfgang Woess, *A survey on spectra of infinite graphs*, Bull. London Math. Soc. **21** (1989), no. 3, 209–234, DOI 10.1112/blms/21.3.209. MR986363 (90d:05162)

[P03] Olaf Post, *Eigenvalues in spectral gaps of a perturbed periodic manifold*, Math. Nachr. **261/262** (2003), 141–162, DOI 10.1002/mana.200310117. MR2020392 (2004m:58052)

[RS78] Michael Reed and Barry Simon, *Methods of modern mathematical physics. IV. Analysis of operators*, Academic Press [Harcourt Brace Jovanovich, Publishers], New York-London, 1978. MR0493421 (58 #12429c)

[S78] Barry Simon, *Classical boundary conditions as a technical tool in modern mathematical physics*, Adv. in Math. **30** (1978), no. 3, 268–281, DOI 10.1016/0001-8708(78)90040-3. MR520236 (80a:81046)

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