SCHRÖDINGER OPERATORS WITH GUIDED POTENTIALS ON PERIODIC GRAPHS

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Abstract. We consider discrete Schrödinger operators with periodic potentials on periodic graphs perturbed by guided non-positive potentials, which are periodic in some directions and finitely supported in other ones. The spectrum of the unperturbed operator is a union of a finite number of non-degenerate bands and eigenvalues of infinite multiplicity. We show that the spectrum of the perturbed operator consists of the unperturbed one plus the additional guided spectrum, which is a union of a finite number of bands. We estimate the position of the guided bands and their length in terms of graph geometric parameters. We also determine the asymptotics of the guided spectrum for large guided potentials. Moreover, we show that the possible number of the guided bands, their length and position can be rather arbitrary for some specific potentials.

1. Introduction

Discrete Schrödinger operators on periodic graphs have attracted a lot of attention due to their applications to the study of electronic properties of real crystalline structures, see, e.g., [Ha02], [H89], [NG04] and the survey [CGPNG09]. Waveguides defects allow one to obtain conductivity of the material for those frequencies (energies) at which it was not in purely periodic structure. Such effects have a lot of applications, see about waveguides in photonic crystal structures in [J00], [JJ02], [H15] and references therein.

We consider discrete Schrödinger operators with periodic potentials on periodic graphs perturbed by guided non-positive potentials, which are periodic in some directions and finitely supported in other ones. For example, on the lattice $\mathbb{Z}^2$ the support of the guided potentials is a strip. It is well-known that the spectrum of Schrödinger operators with periodic potentials on periodic graphs has a band structure with a finite number of flat bands (eigenvalues of infinite multiplicity) [HN09], [HS04], [KS14], [RR07]. The spectrum of the perturbed Schrödinger operator consists of the spectrum of the "unperturbed" operator plus the guided spectrum. The additional guided spectrum is a union of a finite number of bands, here the corresponding wave-functions are located along the support of the guided potentials and decrease in perpendicular directions. Note that line defects on the lattice were considered in [C12], [Ku14], [Ku16], [OA12].

In our paper we study the influence of guided potentials on the spectrum of Schrödinger operators. We describe our main goals:

1) to estimate the position and the length of the guided bands in terms of geometric parameters of graphs and guided potentials;

2) to determine the asymptotics of the guided spectrum for large guided potentials;

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3) to show that the possible number of the guided bands, their length and position can be rather arbitrary for some specific potentials.

1.1. Schrödinger operators with periodic potentials. Let \( \Gamma = (V, E) \) be a connected infinite graph, possibly having loops and multiple edges, where \( V \) is the set of its vertices and \( E \) is the set of its unoriented edges. From the set \( E \) we construct the set \( A \) of oriented edges by considering each edge in \( E \) to have two orientations. An edge starting at a vertex \( u \) and ending at a vertex \( v \) from \( V \) will be denoted as the ordered pair \((u, v) \) \( \in A \). We define the degree \( \kappa_v \) of the vertex \( v \in V \) as the number of all edges from \( A \) starting at \( v \).

Below we consider locally finite \( \mathbb{Z}^\tilde{d} \)-periodic graphs \( \Gamma \), \( \tilde{d} \geq 2 \), i.e., graphs satisfying the following conditions:

1) \( \Gamma \) is equipped with an action of the free abelian group \( \mathbb{Z}^\tilde{d} \);
2) the degree of each vertex is finite;
3) the quotient graph \( \Gamma_\ast = (V_\ast, E_\ast) = \Gamma / \mathbb{Z}^\tilde{d} \) is finite.

We assume that the graphs are embedded into Euclidean space, since in many applications such a natural embedding exists. For example, in the tight-binding approximation real crystalline structures are modeled as discrete graphs embedded into \( \mathbb{R}^d \) \((d = 2, 3) \) and consisting of vertices (points representing positions of atoms) and edges (representing chemical bonding of atoms), by ignoring the physical characters of atoms and bonds that may be different from one another. But all results of the paper stay valid in the case of abstract periodic graphs (without the assumption of graph embedding into Euclidean space).

For a periodic graph \( \Gamma \) embedded into the space \( \mathbb{R}^\tilde{d} \), the quotient graph \( \Gamma / \mathbb{Z}^\tilde{d} \) is a graph on the \( \tilde{d} \)-dimensional torus \( \mathbb{R}^\tilde{d} / \mathbb{Z}^\tilde{d} \). Due to the definition, the graph \( \Gamma \) is invariant under translations through vectors \( a_1, \ldots, a_{\tilde{d}} \) which generate the group \( \mathbb{Z}^\tilde{d} \):

\[
\Gamma + a_s = \Gamma, \quad \forall s \in \mathbb{N}_{\tilde{d}}.
\]

Here and below for each integer \( m \) the set \( \mathbb{N}_m \) is given by

\[
\mathbb{N}_m = \{1, \ldots, m\}. \quad (1.1)
\]

We will call the vectors \( a_1, \ldots, a_{\tilde{d}} \) the periods of the graph \( \Gamma \). In the space \( \mathbb{R}^\tilde{d} \) we consider a coordinate system with the origin at some point \( O \) and with the basis \( a_1, \ldots, a_{\tilde{d}} \). Below the coordinates of all vertices of \( \Gamma \) will be expressed in this coordinate system.

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

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

For a self-adjoint operator \( A \), \( \sigma(A) \), \( \sigma_{\text{ess}}(A) \), \( \sigma_{\text{ac}}(A) \), \( \sigma_p(A) \), and \( \sigma_{f_0}(A) \) denote its spectrum, essential spectrum, absolutely continuous spectrum, point spectrum (eigenvalues of finite multiplicity), and the set of all its flat bands (eigenvalues of infinite multiplicity), respectively.

We consider a discrete Schrödinger operator \( H_0 \) with a periodic potential \( W \) on \( f \in \ell^2(V) \) as an unperturbed operator defined by

\[
H_0 = \Delta + W, \quad (1.2)
\]
where $\Delta$ is the discrete Laplacian (i.e., the combinatorial Laplace operator) given by
\[
(\Delta f)(v) = \sum_{(v,u) \in A} (f(v) - f(u)), \quad \forall f \in \ell^2(V), \quad \forall v \in V,
\] 
and the sum in (1.3) is taken over all oriented edges starting at the vertex $v \in V$. The potential $W$ is real valued and $\mathbb{Z}^d$-periodic, i.e.,
\[
(W f)(v) = W(v) f(v), \quad W(v + a_s) = W(v), \quad \forall (v, s) \in V \times \mathbb{N}_d.
\]

It is well-known that $H_0$ is self-adjoint and its spectrum is a union of $\nu$ spectral bands $\sigma_n(H_0)$:
\[
\sigma(H_0) = \bigcup_{n=1}^\nu \sigma_n(H_0) = \sigma_{ac}(H_0) \cup \sigma_{fb}(H_0), \tag{1.5}
\]
where $\nu = \#V^*$ is the number of vertices of the quotient graph $\Gamma^*$, the absolutely continuous spectrum $\sigma_{ac}(H_0)$ consists of non-degenerate bands $\sigma_n(H_0)$; $\sigma_{fb}(H_0)$ is the set of all flat bands. Without loss of generality assume that the spectrum $\sigma(H_0)$ is a subset of the interval $[0, q]$:
\[
\sigma(H_0) \subset [0, q], \quad \inf \sigma(H_0) = 0, \quad q = \sup \sigma(H_0). \tag{1.6}
\]

1.2. Results overview. There are results about spectral properties of the discrete Schrödinger operator $H_0$ with a periodic potential $W$. The decomposition of the operator $H_0$ into a constant fiber direct integral was obtained in [HN09], [HS04], [RR07] without an exact form of fiber operators and in [KS14], [KS17] with an exact form of fiber operators. In particular, this yields the band-gap structure of the spectrum of the operator $H_0$. In [GKT93] the authors considered the Schrödinger operator with a periodic potential on the lattice $\mathbb{Z}^2$, the simplest example of $\mathbb{Z}^2$-periodic graphs. They studied its Bloch variety and its integrated density of states. In [LP08], [KS15] the positions of the spectral bands of the Laplacians were estimated in terms of eigenvalues of the operator on finite graphs (the so-called eigenvalue bracketing). The estimate of the total length of all spectral bands $\sigma_n(H_0)$
\[
\sum_{n=1}^\nu |\sigma_n(H_0)| \leq 2\beta, \tag{1.7}
\]
was obtained in [KS14]; where $\beta = \#E^* - \nu + 1$ is the so-called Betti number, $\#E^*$ is the number of edges of the quotient graph $\Gamma^*$. Moreover, a global variation of the Lebesgue measure of the spectrum and a global variation of the gap-length in terms of potentials and geometric parameters of the graph were determined. Note that the estimate (1.7) also holds true for magnetic Schrödinger operators with periodic magnetic and electric potentials (see [KS17]). Estimates of the Lebesgue measure of the spectrum of $H_0$ in terms of eigenvalues of Dirichlet and Neumann operators on a fundamental domain of the periodic graph were described in [KS15]. Estimates of effective masses, associated with the ends of each spectral band of the Laplacian, in terms of geometric parameters of the graphs were obtained in [KS16]. Moreover, in the case of the bottom of the spectrum two-sided estimates on the effective mass in terms of geometric parameters of the graphs were determined. The proof of all these results in [KS14]-[KS17] is based on Floquet theory and the exact form of fiber Schrödinger operators from [KS14]. The spectra of the discrete Schrödinger operators on graphene nano-tubes and nano-ribbons in external fields were discussed in [KK10], [KK10a]. Finally, we note that different properties of Schrödinger operators on graphs were considered in [G15], [Sh98].
Scattering theory for self-adjoint Schrödinger operators with decreasing potentials was investigated in [BS99], [IK12] (for the lattice) and in [PR16] (for periodic graphs). Inverse scattering theory with finitely supported potentials was considered in [IK12] for the case of the lattice $\mathbb{Z}^d$ and in [A12] for the case of the hexagonal lattice. The absence of eigenvalues embedded in the essential spectrum of the operators was discussed in [IM14], [V14]. Trace formulae and global eigenvalues estimates for Schrödinger operators with complex decaying potentials on the lattice were obtained in [KL16]. The Cwikel-Lieb-Rosenblum type bound for the discrete Schrödinger operator on $\mathbb{Z}^d$ was computed in [Ka08], [RS09].

2. Main results

2.1. Schrödinger operators with guided potentials. Let integer $d < \tilde{d}$. We define the infinite fundamental graph $\mathcal{C} = \Gamma/\mathbb{Z}^d$ of the $\mathbb{Z}^d$-periodic graph $\Gamma$, which is a graph on the cylinder $\mathbb{R}^d/\mathbb{Z}^d$. We also call the fundamental graph $\mathcal{C}$ a discrete cylinder or just a cylinder. The cylinder $\mathcal{C} = (V_c, \mathcal{E}_c)$ has the vertex set $V_c = V/\mathbb{Z}^d$, the set $\mathcal{E}_c = \mathcal{E}/\mathbb{Z}^d$ of unoriented edges and the set $A_c = A/\mathbb{Z}^d$ of oriented edges. Note that the fundamental graph $\mathcal{C}$ is $\mathbb{Z}^{d-\tilde{d}}$-periodic.

We identify the vertices of the cylinder $\mathcal{C}$ with the vertices of the periodic graph $\Gamma$ from the strip $S = [0, 1)^d \times \mathbb{R}^{d-\tilde{d}}$. We will call this infinite vertex set the fundamental vertex set of $\Gamma$ and denote it by the same symbol $V_c$:

$$V_c = V \cap S, \quad S = [0, 1)^d \times \mathbb{R}^{d-\tilde{d}}. \quad (2.1)$$

Edges of the periodic graph $\Gamma$ connecting the vertices from the fundamental vertex set $V_c$ with the vertices from $V \setminus V_c$ will be called bridges. Bridges always exist and provide the connectivity of the periodic graph. The set of all bridges of the graph $\Gamma$ we denote by $\mathcal{B}$.

We consider a guided Schrödinger operator $H$ on the periodic graph $\Gamma$ given by

$$H = H_0 - Q, \quad (Qf)(v) = Q(v)f(v), \quad f \in \ell^2(V), \quad (2.2)$$

where $Q$ is the guided potential defined by

1) $Q \geq 0$ and $Q$ is $\mathbb{Z}^d$-periodic, i.e.,

$$Q(v + a_s) = Q(v), \quad \forall (v,s) \in V_c \times \mathbb{N}_d, \quad (2.3)$$

2) the restriction of $Q$ to $V_c$ has a finite support:

$$\text{supp}(Q|V_c) = \{v_1, \ldots, v_p\} \subset V_c. \quad (2.4)$$

In other words, the guided potential $Q$ is periodic in the directions $a_1, \ldots, a_d$ and finitely supported in other ones, see Fig.1.

Example. For the square lattice $\mathbb{L}^2$ with the periods $a_1, a_2$, see Fig.1.a, the discrete cylinder $\mathcal{C} = \mathbb{L}^2/\mathbb{Z} = (V_c, \mathcal{E}_c)$ is shown in Fig.1.b. The vertices from the set $V_c$ are big black points. The guided potential $Q$ is shown by vertical lines. The spectrum of a guided operator on the square lattice $\mathbb{L}^2$ is discussed in Example 3.1.

We define the torus $\mathbb{T}^d = \mathbb{R}^d/(2\pi \mathbb{Z})^d$ and describe the basic spectral properties of guided Schrödinger operators.

Proposition 2.1. i) The guided Schrödinger operator $H = H_0 - Q$ has the following decomposition into a constant fiber direct integral for some unitary operator $U : \ell^2(V) \to \mathscr{H}$:

$$\mathscr{H} = \int_{\mathbb{T}^d} \ell^2(V_c) \frac{d\vartheta}{(2\pi)^d}, \quad \mathbb{U}^{-1} = \int_{\mathbb{T}^d} H(\vartheta) \frac{d\vartheta}{(2\pi)^d}, \quad H(\vartheta) = H_0(\vartheta) - Q, \quad (2.5)$$
where the fiber Schrödinger operator $H(\vartheta)$ acts on the fiber space $\ell^2(V_c)$ and $H_0(\vartheta) = \Delta(\vartheta) + W$ is the fiber operator for $H_0$, the fiber Laplacian $\Delta(\vartheta)$ is given by

$$
(\Delta(\vartheta) f)(v) = \sum_{e=(v, u) \in A_c} (f(v) - e^{i(\tau(e), \vartheta)} f(u)), \quad v \in V_c, \quad f \in \ell^2(V_c),
$$

(2.6)

the potential $Q$ on $\ell^2(V_c)$ has a finite rank. Here $\tau(e) \in \mathbb{Z}^d$ is the index of the edge $e \in A_c$ defined by (3.2) and (3.3), $V_c$ and $A_c$ are the vertex set and the set of oriented edges of the cylinder $C$, respectively; $\langle \cdot, \cdot \rangle$ is the inner product in $\mathbb{R}^d$.

ii) For each $\vartheta \in \mathbb{T}^d$ the spectrum of the fiber operator $H(\vartheta)$ has the form

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

(2.7)

$$
\sigma_{ac}(H(\vartheta)) = \sigma_{ac}(H_0(\vartheta)), \quad \sigma_{fb}(H(\vartheta)) = \sigma_{fb}(H_0(\vartheta)),
$$

(2.8)

$\sigma_p(H(\vartheta))$ is the set of all eigenvalues of $H(\vartheta)$ of finite multiplicity given by

$$
\lambda_1(\vartheta) \leq \lambda_2(\vartheta) \leq \ldots \leq \lambda_{N_\vartheta}(\vartheta), \quad N_\vartheta \leq p = \text{rank}(Q | V_c).
$$

(2.9)

Remark. The fiber Laplacian $\Delta(\vartheta)$, $\vartheta \in \mathbb{T}^d$, can be considered as a magnetic Laplacian with a periodic magnetic potential on the cylinder $C$ (see [HS99a], [HS99b], [KS17]).

Proposition 2.1 and standard arguments (see Theorem XIII.85 in [RS78]) describe the spectrum of the guided Schrödinger operator $H$. Since $H(\vartheta)$ is self-adjoint and analytic in $\vartheta \in \mathbb{T}^d$, each $\lambda_j(\cdot)$ is a real and piecewise analytic function on the torus $\mathbb{T}^d$ and creates the guided band $s_j(H)$ given by

$$
s_j(H) = [\lambda_j^-, \lambda_j^+] = \lambda_j(\mathbb{T}^d), \quad j = 1, \ldots, N, \quad N = \max_{\vartheta \in \mathbb{T}^d} N_\vartheta \leq p.
$$

(2.10)

Thus, the spectrum of the guided Schrödinger operator $H$ on the graph $\Gamma$ has the form

$$
\sigma(H) = \bigcup_{\vartheta \in \mathbb{T}^d} \sigma(H(\vartheta)) = \sigma(H_0) \cup s(H),
$$

where $\sigma(H_0)$ is defined by (1.5) and

$$
s(H) = \bigcup_{\vartheta \in \mathbb{T}^d} \sigma_p(H(\vartheta)) = \bigcup_{j=1}^N s_j(H) = s_{ac}(H) \cup s_{fb}(H),
$$

(2.11)
s_{ac}(H) and s_{fb}(H) are the absolutely continuous part and the flat band part of the guided spectrum \( s(H) \), respectively. An open interval between two neighboring non-degenerate bands is called a spectral gap. The guided spectrum \( s(H) \) may partly lie below the spectrum of the unperturbed operator \( H_0 \), on the spectrum of \( H_0 \) and in the gaps of \( H_0 \).

### 2.2. Estimates of guided bands

We consider the guided bands from \((2.10)\) (or their parts) below the spectrum of the unperturbed Schrödinger operator \( H_0 \), i.e., below \( \inf \sigma(H_0) = 0 \):

\[
s_j^g(H) = s_j(H) \cap (-\infty, 0] \neq \emptyset, \quad j = 1, \ldots, N_g, \quad N_g \leq N. \tag{2.11}
\]

We rewrite the sequence \( Q(v), v \in \text{supp}(Q \mid V_c) \) in the form

\[
0 < Q_{p}^* \leq \ldots \leq Q_{2}^* \leq Q_{1}^*, \tag{2.12}
\]

where \( Q_j^* = Q(v_j), j = 1, \ldots, p \), for some distinct vertices \( v_1, v_2, \ldots, v_p \in \text{supp}(Q \mid V_c) \).

Proposition \([2.1]\) and the standard perturbation theory give the estimates of the position of the bands \( s_j^g(H) \) and their number \( N_g \) by

\[
s_j^g(H) \subset [-Q_j^*, -Q_j^* + \varrho], \quad N_g \geq \# \{ j \in \mathbb{N}_p : Q_j^* > \varrho \}, \tag{2.13}
\]

where \( \varrho \) is defined in \((1.6)\) (for more details see Corollary \([4.1]\) \#A is the number of elements of the set \( A \). In particular, this yields that the guided spectrum may lie below any fixed point and for guided potentials \( Q \) satisfying \( Q_{p}^* > \varrho \) and \( Q_{j+1}^* - Q_{j}^* > \varrho \) for all \( j \in \mathbb{N}_p \) the guided spectrum of \( H = H_0 - Q \) consists of exactly \( p \) guided bands separated by gaps.

In order to formulate our main result we define the set \( B_c = \mathcal{B} / \mathbb{Z}^d \) of all bridges of the cylinder \( C = (V_c, E_c) \) and the modified cylinder \( C_m = (V_c, E_c \setminus B_c) \), which is obtained from \( C \) by deleting all its bridges. We consider the Schrödinger operator \( h \) on the modified cylinder \( C_m \):

\[
h = h_0 - Q, \quad h_0 = \Delta_m + W. \tag{2.14}
\]

Here \( \Delta_m \) is the Laplacian defined by \((1.3)\) on the cylinder \( C_m \) and \( W \) is the restriction of the periodic potential defined by \((1.4)\) to the vertex set \( V_c \). The potential \( Q \) has a finite support \( \{ v_1, \ldots, v_p \} \) on the cylinder \( C_m \). Then the Schrödinger operator \( h \) has at most \( p = \text{rank} Q \) eigenvalues \( \tilde{\mu}_1 \leq \tilde{\mu}_2 \leq \ldots \). Define \( \mu_j \) by

\[
\mu_j = \min \{ \tilde{\mu}_j, \inf \sigma_{ess}(h) \}, \quad j = 1, 2, \ldots, p. \tag{2.15}
\]

We estimate the position of the guided bands \( s_j^g(H) \) defined by \((2.11)\) in terms of the eigenvalues of the operator \( h \) and the number of bridges on the cylinder \( C \).

**Theorem 2.2.** Let \( H = H_0 - Q \) be a guided Schrödinger operator. Then each guided band \( s_j^g(H), j = 1, \ldots, N_g, \) defined by \((2.11)\) satisfies

\[
s_j^g(H) \subset [\mu_j, \mu_j + 2\beta_+], \quad \beta_+ = \max_{v \in V_c} \beta_v, \tag{2.16}
\]

where \( \beta_v \) denotes the number of bridges on \( C \) starting at the vertex \( v \in V_c \).

**Remarks.** 1) For most of graphs the number \( \beta_+ = 1 \) and, consequently, the length of each guided band \( |s_j^g(H)| \leq 2, j = 1, \ldots, N_g \). But for specific graphs \( \beta_+ \) may be any given integer number.

2) Note that there exists a periodic graph \( \Gamma \) such that the inclusions \((2.10)\) become identities and \( |s_j^g(H)| = 2\beta_+, j = 1, \ldots, N_g, \) for any guided potential \( Q \), see Example \([3.1]\).

We discuss the guided spectrum in the case of the guided potentials large enough.
Theorem 2.3. Let $H_t = \Delta + W - tQ$ be a guided Schrödinger operator, where the coupling constant $t > 0$ is large enough. Then $N_p = p$ and the following statements hold true:

i) Let $Q_j^* \neq Q_k^*$ for some fixed $j \in \mathbb{N}_p$ and all $k \in \mathbb{N}_p \setminus \{j\}$. Then the guided band $s_j(H_t) = [\lambda_j^-(t), \lambda_j^+(t)]$ satisfies

$$
\lambda_j^+(t) = -tQ_j^* + W(v_j) + \Delta_j^+ + O(1/t),
$$

$$
|s_j(H_t)| = \Delta_j + O(1/t),
$$

as $t \to \infty$, where

$$
\Delta_j^\pm = \min_{\vartheta \in \mathbb{T}^d} \Delta_{jj}(\vartheta) - \nu_{v_j}, \quad \Delta_j^\pm = \max_{\vartheta \in \mathbb{T}^d} \Delta_{jj}(\vartheta),
$$

for some function $\Delta_{jj}(\vartheta)$ defined by the formula (4.12). Here $\nu_{v_j}$ is the degree of the vertex $v_j \in \text{supp}(Q \mid V_c)$, $\nu_{q_{jj}}$ is the number of all oriented bridge-loops at this vertex on the cylinder $\mathbb{C}$ and $\nu_{q_{jj}}$ is the number of the remaining oriented loops at $v_j$ on $\mathbb{C}$.

ii) Let $Q$ be "generic", i.e., $Q_j \neq Q_k$ for all $j, k \in \mathbb{N}_p, k \neq j$. Then the Lebesgue measure $|s(H_t)|$ of the guided spectrum of the operator $H_t$ satisfies

$$
|s(H_t)| = \sum_{j=1}^{p} \Delta_j + O(1/t).
$$

iii) In particular, if there exists a bridge-loop at a vertex $v_j \in \text{supp}(Q \mid V_c)$ on the cylinder $\mathbb{C}$, then $\Delta_j \neq 0$ and the guided band $s_j(H_t)$ is non-degenerate. If there are no such bridge-loops at $v_j$, then $\Delta_j = 0$ and $|s_j(H_t)| = O(1/t)$. Moreover, if there are no bridge-loops at each vertex $v \in \text{supp}(Q \mid V_c)$ on $\mathbb{C}$, then $|s(H_t)| = O(1/t)$.

Remark. There exist periodic graphs $\Gamma$ and guided potentials $Q$ such that the Lebesgue measure of the guided spectrum of $H = H_0 - Q$ on $\Gamma$ can be arbitrarily large or arbitrarily small (for more details see Corollary 4.2).

We present the plan of our paper. In Section 3 we prove Proposition 2.1 about the decomposition of guided Schrödinger operators into a constant fiber direct integral. In Section 4 we prove Theorem 2.2 describing the localization of the guided bands and Theorem 2.3 about the asymptotics of the guided bands for large guided potentials and finally describe geometric properties of the guided spectrum for specific graphs and guided potentials.

3. Direct integral for guided Schrödinger operators

3.1. Edge indices. In order to give a decomposition of guided Schrödinger operators into a constant fiber direct integral with a precise representation of fiber operators we need to define an edge index. Recall that an edge index was introduced in [KS14] and it was important to study the spectrum, effective masses of Laplacians and Schrödinger operators on periodic graphs, since fiber operators are expressed in terms of edge indices (see (2.6)).

For any $v \in V$ the following unique representation holds true:

$$
v = v_0 + [v], \quad v_0 \in V_c, \quad [v] \in \mathbb{Z}^d,
$$

where $V_c$ is the fundamental vertex set of the periodic graph $\Gamma$ defined by (2.1). In other words, each vertex $v$ can be obtained from a vertex $v_0 \in V_c$ by the shift by a vector $[v] \in \mathbb{Z}^d$. 
For any oriented edge $e = (u, v) \in \mathcal{A}$ we define the edge "index" $\tau(e)$ as the integer vector given by

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

(3.2)

where, due to (3.1), we have

$$u = u_0 + [u], \quad v = v_0 + [v], \quad u_0, v_0 \in V_c, \quad [u], [v] \in \mathbb{Z}^d.$$ 

We note that edges connecting vertices from the fundamental vertex set given by

$$\Delta$$

If

$$Q$$

standard arguments (see Theorem XIII.85 in [RS78]), we obtain that the spectrum of

$$C$$

Let

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For any oriented edge $e \in \mathcal{A}$, if $e$ is an oriented edge of the graph $\Gamma$, then there is an oriented edge $e_\ast = f_\mathcal{A}(e)$ on the cylinder $C = \Gamma/\mathbb{Z}^d$. For the edge $e_\ast \in \mathcal{A}_c$ we define the edge index $\tau(e_\ast)$ by

$$\tau(e_\ast) = \tau(e).$$

(3.3)

In other words, edge indices of the cylinder $C$ are induced by edge indices of the periodic graph $\Gamma$. Edges with nonzero indices are called bridges. Edge indices, generally speaking, depend on the choice of the coordinate origin $O$ and the periods $a_1, \ldots, a_7$ of the graph $\Gamma$. But in a fixed coordinate system indices of the cylinder edges are uniquely determined by (3.3), since

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

3.2. Direct integrals and an example of the guided spectrum. We prove Proposition 2.1 about the decomposition of guided Schrödinger operators into a constant fiber direct integral and give an example of the guided spectrum.

Proof of Proposition 2.1. i) Repeating the arguments from the proof of Theorem 1.1 in [KL14] we obtain (2.5), (2.6), where the unitary operator $U : \ell^2(V) \to \mathcal{H}$ has the form

$$\langle Uf \rangle(\vartheta, v) = \sum_{m \in \mathbb{Z}^d} e^{-i(m, 0)} f(v + m), \quad (\vartheta, v) \in \mathbb{T}^d \times V_c, \quad f \in \ell^2(V).$$

(4.4)

The Hilbert space $\mathcal{H}$ defined in (2.5) is equipped with the norm $\|g\|^2_{\mathcal{H}} = \int_{\mathbb{T}^d} \|g(\vartheta, \cdot)\|^2_{\ell^2(V_c)} d\vartheta$, where the function $g(\vartheta, \cdot) \in \ell^2(V_c)$ for almost all $\vartheta \in \mathbb{T}^d$. The fiber potential $Q$ is a finite rank operator, since $\text{supp}(Q | V_c) = \{v_1, \ldots, v_p\} \subset V_c$ is finite.

ii) For each $\vartheta \in \mathbb{T}^d$ the unperturbed fiber operator $H_0(\vartheta)$ is $\mathbb{Z}^d$-periodic. Then, using standard arguments (see Theorem XIII.85 in [RS78]), we obtain that the spectrum of $H_0(\vartheta)$ has the form

$$\sigma(H_0(\vartheta)) = \sigma_{ac}(H_0(\vartheta)) \cup \sigma_{fb}(H_0(\vartheta)).$$

Since the fiber potential $Q$ is an operator of rank $p = \text{# supp}(Q | V_c)$, for each $\lambda \in \sigma_{fb}(H_0(\vartheta))$ there exists a corresponding eigenfunction with a finite support (see, e.g., Theorem 4.5.2 in [BK13]) not intersecting with $\text{supp}(Q | V_c)$. Thus, $\lambda \in \sigma_{fb}(H(\vartheta))$ and vice versa. Then for each $\vartheta \in \mathbb{T}^d$ the spectrum $\sigma(H(\vartheta))$ of the fiber operator $H(\vartheta)$ is given by (2.7), where $\sigma_{ac}(H(\vartheta)), \sigma_{fb}(H(\vartheta))$ satisfy (2.8) and $\sigma_p(H(\vartheta))$ consists of $N_\vartheta \leq p$ eigenvalues (2.9). ■

We consider a simple example of the guided spectrum.

Example 3.1. Let $L^2 = (V, \mathcal{E})$ be the square lattice, where the vertex set $V = \mathbb{Z}^2$ and the edge set $\mathcal{E} = \{(m, m + a_s), \forall m \in \mathbb{Z}^2, s = 1, 2\}$ and $a_1 = (1, 0), a_2 = (0, 1)$, see Fig 2a. Our Laplacian $\Delta$ defined by (1.3) has the form

$$\langle \Delta f \rangle(m) = 4f(m) - \sum_{|m-k|=1} f(k), \quad f \in \ell^2(\mathbb{Z}^2), \quad m \in \mathbb{Z}^2.$$ 

3.5
We consider a Schrödinger operator $H = \Delta - Q$ on $\mathbb{Z}^2$, where $Q \geq 0$ is a guided potential such that

$$(Qf)(m) = Q(m_2)f(m), \quad m = (m_1, m_2),$$

and $Q(m_2)$ is finitely supported on $\mathbb{Z}$.

Due to Proposition 2.1, the guided operator $H = \Delta - Q$ on the lattice $\mathbb{Z}^2$ has the decomposition (2.5) into a constant fiber direct integral, where the fiber Schrödinger operator $H(\vartheta) = \Delta(\vartheta) - Q$ acts on $f \in \ell^2(\mathbb{Z})$ and is given by

$$H(\vartheta) = 2(1 - \cos \vartheta) + h,$$

$$hf(n) = 2f(n) - f(n+1) - f(n-1) - Q(n)f(n), \quad n \in \mathbb{Z}, \quad (3.6)$$

for all $\vartheta \in \mathbb{T} = (-\pi, \pi]$. The operator $h$ is well studied, see [T89] for a large class of $Q$, and see [K11] in the case of finitely supported $Q$, where the inverse problem is solved. It is well known that the spectrum of the operator $h$ consists of an absolutely continuous part $[0, 4]$ plus a finite number of simple eigenvalues

$$\mu_1 < \mu_2 < \ldots < \mu_N < 0, \quad N \leq p, \quad p = \text{rank} Q.$$

Then, each fiber operator $H(\vartheta)$, $\vartheta \in \mathbb{T}$, has at most $p$ simple eigenvalues:

$$\lambda_1(\vartheta) < \lambda_2(\vartheta) < \ldots < \lambda_N(\vartheta) < 2 - 2\cos \vartheta, \quad \text{where} \quad \lambda_j(\vartheta) = \mu_j + 2 - 2\cos \vartheta, \quad j \in \mathbb{N}_N.$$

Thus, the definition (2.10) of the guided bands $s_j(H)$ yields

$$s_j(H) = \lambda_j(\mathbb{T}) = [\mu_j, \mu_j + 4], \quad |s_j(H)| = 4, \quad j \in \mathbb{N}_N, \quad N \leq p.$$

On the other hand, the number $\beta_+$ defined in (2.16) is equal to 2, since for each vertex of the cylinder $C$ there are two bridges starting at this vertex. Thus, on the graph $\mathbb{L}^2$ the inclusions (2.16) become identities. $\blacklozenge$

4. Proof of the main results

In this section we prove Theorem 2.2 about the position of the guided bands and Theorem 2.3 about the asymptotics of the guided bands for large guided potentials. We also describe geometric properties of the guided spectrum for specific graphs and guided potentials (see Corollary 4.2).
4.1. Estimates for the guided spectrum. Denote by $m_\pm(\vartheta)$ the upper and lower endpoints of the spectrum of the unperturbed fiber operator $H_0(\vartheta)$:

$$
m_-(\vartheta) = \inf \sigma(H_0(\vartheta)), \quad m_+(\vartheta) = \sup \sigma(H_0(\vartheta)).
$$

Then (1.6) yields

$$
\min_{\vartheta \in \mathbb{T}^d} m_-(\vartheta) = 0, \quad \max_{\vartheta \in \mathbb{T}^d} m_+(\vartheta) = \varrho.
$$

We need a simple estimate for eigenvalues of bounded self-adjoint operators [RS78]: Let $A, B$ be bounded self-adjoint operators in a Hilbert space $\mathcal{H}$ and let $\lambda_j(A) = \min \{\tilde{\lambda}_j(A), \inf \sigma_{ess}(A)\}$, $j = 1, 2, \ldots$, where $\tilde{\lambda}_1(A) \leq \tilde{\lambda}_2(A) \leq \ldots$ are the eigenvalues of $A$. Then

$$
\lambda_j(A) + \inf \sigma(B) \leq \lambda_j(A + B) \leq \lambda_j(A) + \sup \sigma(B), \quad j = 1, 2, 3, \ldots.
$$

The following simple corollary about the position of the guided bands $\mathfrak{s}_j^\vartheta(H)$ defined by (2.11) is a direct consequence of Proposition 2.1.

**Corollary 4.1.** Let $H = H_0 - Q$ be a guided Schrödinger operator and let $\varrho$ be defined in (1.6). Then each guided band $\mathfrak{s}_j^\vartheta(H)$, $j = 1, \ldots, N_g$, and their number $N_g$ satisfy

$$
\mathfrak{s}_j^\vartheta(H) \subset [-Q_j^\vartheta, -Q_j^\vartheta + \varrho],
$$

$$
N_g \geq \#\{j \in \mathbb{N}_p : Q_j^\vartheta > \varrho\}.
$$

**Proof.** The fiber Schrödinger operator $H(\vartheta)$ is given by $H(\vartheta) = H_0(\vartheta) - Q$, $Q \geq 0$. Then, due to (4.3), (4.1) and (4.2), for each $\vartheta \in \mathbb{T}^d$ the eigenvalues $\lambda_j(\vartheta)$ of $H(\vartheta)$ below its essential spectrum satisfy

$$
-Q_j^\vartheta \leq m_-(\vartheta) - Q_j^\vartheta \leq \lambda_j(\vartheta) \leq m_+(\vartheta) - Q_j^\vartheta \leq \varrho - Q_j^\vartheta,
$$

which yields (4.4). Let $Q_j^\vartheta > \varrho$ for some $j = 1, \ldots, p$. Then, due to (1.6), $\lambda_j(\vartheta) < 0$ for all $\vartheta \in \mathbb{T}^d$. Thus, $\lambda_j$ creates the guided band $\mathfrak{s}_j^\vartheta(H) = \lambda_j(\mathbb{T}^d)$. This yields (4.5). $\blacksquare$

**Proof of Theorem 2.2.** We rewrite the fiber operator $H(\vartheta)$, $\vartheta \in \mathbb{T}^d$, defined by (2.5), (2.6) in the form:

$$
H(\vartheta) = h + \Delta_\beta(\vartheta), \quad h = \Delta_m + W - Q,
$$

$$
(\Delta_\beta(\vartheta)f)(v) = \sum_{e=(v, w) \in \mathcal{A}_\vartheta} (f(v) - e^{i(\tau(e), \vartheta)} f(u)), \quad v \in V_c,
$$

where $\tau(e) \in \mathbb{Z}^d$ is the index of the edge $e \in \mathcal{A}_\vartheta$ defined by (3.2), (3.3). Each operator $\Delta_\beta(\vartheta)$, $\vartheta \in \mathbb{T}^d$, is the magnetic Laplacian on the graph $\mathcal{C}_\beta = (V_c, \mathcal{B}_c)$ and the degree of each vertex $v \in V_c$ on $\mathcal{C}_\beta$ is equal to the number $\beta_v$ of all bridges starting at $v$. Then the spectrum of $\Delta_\beta(\vartheta)$ satisfies

$$
\sigma(\Delta_\beta(\vartheta)) \subset [0, 2\beta_+], \quad \forall \vartheta \in \mathbb{T}^d
$$

(see, e.g., [HS99a], [HS99b]) and, due to (4.3), we have $\mu_j \leq \lambda_j(\vartheta) \leq \mu_j + 2\beta_+$ for each $\vartheta \in \mathbb{T}^d$ and each $j = 1, \ldots, N_g$, which yields (2.16). $\blacksquare$
4.2. Proof of Theorem 2.3. We consider the guided Schrödinger operator \( H_t = H_0 - tQ \), \( Q \gg 0 \). If \( t > 0 \) is large enough, then \( tQ_j^* > \rho \) for each \( j = 1, \ldots, p \), where \( \rho \) is defined in (1.6). Then, due to (4.5) and the inequality \( N_g \leq p \), we have \( N_g = p \).

i) We rewrite the fiber operator \( H_t(\vartheta) \), \( \vartheta \in \mathbb{T}^d \), for the guided operator \( H_t \) in the form

\[
H_t(\vartheta) = H_0(\vartheta) - tQ = tK_t(\vartheta), \quad K_t(\vartheta) = -Q + \varepsilon H_0(\vartheta), \quad \varepsilon = \frac{1}{t}.
\]

We denote the eigenvalues of the operator \( K_t(\vartheta) \) below its essential spectrum by

\[
E_1(\vartheta, t) \leq E_2(\vartheta, t) \leq \ldots \leq E_p(\vartheta, t), \quad \vartheta \in \mathbb{T}^d.
\]

For each vertex \( u \in \text{supp}(Q \upharpoonright V_c) \) we define the function \( f_u \in \ell^2(V_c) \) by \( f_u(v) = \delta_{uv} \), where \( \delta_{uv} \) is the Kronecker delta. Then the eigenvalue \( E_j(\vartheta, t) \) of the operator \( K_t(\vartheta) \) has the following asymptotics:

\[
E_j(\vartheta, t) = -Q_j^* + \varepsilon \langle f_{v_j}, H_0(\vartheta)f_{v_j}\rangle_{V_c} + \varepsilon^2 \sum_{k=1}^{p} \frac{|\langle f_{v_k}, H_0(\vartheta)f_{v_j}\rangle_{V_c}|^2}{Q_k^* - Q_j^*} + O(\varepsilon^3)
\]

(see pp. 7–8 in [RS78]) uniformly in \( \vartheta \in \mathbb{T}^d \) as \( t \to \infty \), where \( \langle \cdot, \cdot \rangle_{V_c} \) denotes the inner product in \( \ell^2(V_c) \). Using the identity \( H_0(\vartheta) = \Delta(\vartheta) + W \) and the formula (2.6) for the fiber Laplacian \( \Delta(\vartheta) \), we rewrite the asymptotics (4.10) in the form

\[
E_j(\vartheta, t) = -Q_j^* + \varepsilon (\Delta_{jj}(\vartheta) + W(v_j)) + O(\varepsilon^2),
\]

where \( \Delta_{jj}(\vartheta) \) is defined by

\[
\Delta_{jj}(\vartheta) = \kappa_j - \sum_{e=(v_j, v_j) \in \mathcal{A}_c} \cos(\tau(e), \vartheta).
\]

Here \( \kappa_e \) is the degree of the vertex \( v \), the vertices \( v_1, v_2, \ldots, v_p \in \text{supp}(Q \upharpoonright V_c) \) and \( \tau(e) \in \mathbb{Z}^d \) is the edge index defined by (3.2), (3.3). This yields the asymptotics of the eigenvalue \( \lambda_j(\vartheta, t) \) of the operator \( H_t(\vartheta) \):

\[
\lambda_j(\vartheta, t) = t E_j(\vartheta, t) = -Q_j^* + \Delta_{jj}(\vartheta) + W(v_j) + O(1/t).
\]

Using this asymptotics for \( \lambda_j^-(t) = \min_{\vartheta \in \mathbb{T}^d} \lambda_j(\vartheta, t) \) and \( \lambda_j^+(t) = \max_{\vartheta \in \mathbb{T}^d} \lambda_j(\vartheta, t) \), we obtain

\[
\lambda_j^+(t) = -tQ_j^* + \Delta_j^+ + W(v_j) + O(1/t),
\]

where \( \Delta_j^\pm \) are defined in (2.18). Since \( \mathcal{S}_j(H_t) = [\lambda_j^-(t), \lambda_j^+(t)] \), the asymptotics (4.13) also gives the second formula in (2.17). Using (4.12) we rewrite the constant \( \Delta_j \) defined in (2.18) in the form

\[
\Delta_j = \max_{\vartheta \in \mathbb{T}^d} \Omega_j(\vartheta) - \min_{\vartheta \in \mathbb{T}^d} \Omega_j(\vartheta) = \beta_{jj} - \min_{\vartheta \in \mathbb{T}^d} \Omega_j(\vartheta), \quad \Omega_j(\vartheta) = \sum_{e=(v_j, v_j) \in \mathcal{A}_c} \cos(\tau(e), \vartheta).
\]

Using the identity \( \int \cos(\tau(e), \vartheta) \, d\vartheta = 0 \) for each \( \tau(e) \neq 0 \), we obtain \( -\beta_{jj} \leq \min_{\vartheta \in \mathbb{T}^d} \Omega_j(\vartheta) \leq 0 \) and (4.14) yields \( \beta_{jj} \leq \Delta_j \leq 2\beta_{jj} \).

ii) If the guided potential \( Q \) is generic, then summing the second asymptotics in (2.17) over \( j = 1, \ldots, p \) we obtain (2.19).

iii) Let on the cylinder \( \mathcal{C} \) there exist a bridge-loop at a vertex \( v_j \in \text{supp}(Q \upharpoonright V_c) \), i.e., a loop \( e \) with \( \tau(e) \neq 0 \). This yields that the function \( \Delta_{jj} \) defined by (4.12) is not constant, i.e., \( \Delta_j \neq 0 \),
and, due to the second asymptotics in (2.17), the guided band $s_j(H_t)$ is non-degenerate. If there are no bridge-loops at $v_j$ on $C$, then $\Delta_{jj}$ is constant, i.e., $\Delta_j = 0$, and, using the second asymptotics in (2.17), we obtain $|s_j(H_t)| = O(1/t)$.

If for each $v \in \text{supp}(Q \upharpoonright V_c)$ there are no bridge-loops at $v$ on $C$, then $\Delta_j = 0$ for each $j \in \mathbb{N}_p$, and the asymptotics (2.19) takes the form $|s(H_t)| = O(1/t)$.

**Remarks.**  
1) The set $A_c$ of all oriented edges of the cylinder $C$ is infinite, but the sum in (4.12) is taken over a finite (maybe empty) set of edge-loops at the vertex $v_j$.

2) If all bridge-loops at some vertex $v_j \in \text{supp}(Q \upharpoonright V_c)$ on $C$ have linearly independent indices, then $\Delta_j$ defined in (2.18) is equal to $2\beta_{jj}$.

Now we describe geometric properties of the guided spectrum for specific graphs and guided potentials.

**Corollary 4.2.** Let $H = H_0 - Q$ be a guided Schrödinger operator. Then the following statements hold true.

1) Let there exist a bridge-loop on the cylinder $C$. Then for any constant $C > 0$ there exists a guided potential $Q \geq 0$ such that the Lebesgue measure of the guided spectrum $s(H)$ satisfies $|s(H)| > C$ and all guided bands are non-degenerate.

2) Let there exist a vertex $v \in V_c$ such that there is no bridge-loop at $v$ on $C$. Then for any small $\varepsilon > 0$ there exists a guided potential $Q \geq 0$ such that the Lebesgue measure of the guided spectrum $s(H)$ satisfies $|s(H)| < \varepsilon$.

**Remark.** An example of a cylinder $C$ with bridge-loops is shown in Fig. 2.

**Proof.** We consider guided Schrödinger operators $H_t = H_0 - tQ$, $Q \geq 0$ with the coupling constant $t > 0$ large enough. Due to Theorem 2.3, the number $N_g$ of the guided bands $s_j^g(H_t) = s_j(H_t)$ is equal to $p$.

1) Let $e_{1q}, \ldots, e_{1q} \in A_c$ be all bridge-loops at some vertex $v_1 \in V_c$ and $\tau(e_{11}), \ldots, \tau(e_{1q})$ be their indices defined by (3.2), (3.3). Due to the periodicity of the cylinder $C$, at each vertex $v_j = v_1 + (j - 1)a_\Delta$, $j \in \mathbb{Z}$, there exist exactly $q$ bridge-loops $e_{j1}, \ldots, e_{jq} \in A_c$ with the same indices $\tau(e_{j1}), \ldots, \tau(e_{jq})$. Then we have

$$\Delta_{11}(\theta) = \Delta_{22}(\theta) = \ldots, \quad (4.15)$$

where $\Delta_{jj}$ is defined by (4.12).

Let $Q$ be a ”generic” guided potential, i.e., $Q_j \neq Q_k$ for all $j, k \in \mathbb{N}_p$, $j \neq k$, with $\text{supp}(Q \upharpoonright V_c) = \{v_1, v_2, \ldots, v_p\}$ for some $p \in \mathbb{N}$. Then, due to Theorem 2.3 for $t$ large enough the guided bands $s_j(H_t)$, $j = 1, \ldots, p$, satisfy

$$|s_j(H_t)| = \Delta_j + O(1/t),$$

where $\Delta_j$ is defined in (2.18) and, due to (4.15), the constant $\Delta_j \neq 0$ is the same for all $j = 1, \ldots, p$. This yields that all guided bands are non-degenerate and

$$|s(H_t)| = \sum_{j=1}^{p} |s_j(H_t)| = p \Delta_1 + O(1/t). \quad (4.16)$$

Choosing $p > \frac{C}{\Delta_1}$, we obtain $|s(H_t)| > C$ for $t$ large enough.
ii) Let there exist a vertex $v \in V_c$ such that there is no bridge-loop at $v$ on $C$. We consider the guided potential $Q$ with $\text{supp}(Q|_{V_c}) = \{v\}$. Due to Theorem 2.3, for $t$ large enough the guided spectrum of $H_t$ consists of exactly one guided band $s_1(H_t)$ and the length of this guided band satisfies $|s_1(H_t)| = O(1/t)$. Thus, for any small $\varepsilon > 0$ there exists $t > 0$ such that $|s(H_t)| < \varepsilon$. 

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