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Schrödinger operators on periodic discrete graphs

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A B S T R A C T

We consider Schrödinger operators with periodic potentials on periodic discrete graphs. The spectrum of the Schrödinger operator consists of an absolutely continuous part (a union of a finite number of non-degenerated bands) plus a finite number of flat bands, i.e., eigenvalues of infinite multiplicity. We obtain estimates of the Lebesgue measure of the spectrum in terms of geometric parameters of the graph and show that they become identities for some class of graphs. Moreover, we obtain stability estimates and show the existence and positions of large number of flat bands for specific graphs. The proof is based on the Floquet theory and the precise representation of fiber Schrödinger operators, constructed in the paper.

Contents

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1. Introduction

We discuss the spectral properties of both Laplacians and Schrödinger operators with periodic potentials on $\mathbb{Z}^d$-periodic discrete graphs, $d \geqslant 2$. Schrödinger operators on periodic graphs are of interest due to their applications to problems of physics and chemistry. They are used to study properties of different periodic media, e.g. nanomedia, see [12,31] and a nice survey [6].

There are a lot of papers, and even books, on the spectrum of discrete Laplacians on finite and infinite graphs (see [4,8–10,33] and references therein). There are results about spectral properties of discrete Schrödinger operators on specific $\mathbb{Z}^d$-periodic graphs. Schrödinger operators with decreasing potentials on the lattice $\mathbb{Z}^d$ are considered by Boutet de Monvel and Sahbani [5], Isozaki and Korotyaev [16], Rosenblum and Solomjak [36] and see references therein. Ando [1] considers the inverse spectral theory for the discrete Schrödinger operators with finitely supported potentials on the hexagonal lattice. Gieseker, Knörrer and Trubowitz [11] consider Schrödinger operators with periodic potentials on the lattice $\mathbb{Z}^2$, the simplest example of $\mathbb{Z}^2$-periodic graphs. They study its Bloch variety and its integrated density of states. Korotyaev and Kutsenko [19–21] study the spectra of the discrete Schrödinger operators on graphene nano-tubes and nano-ribbons in external fields.

We describe the main goals of our paper:

1) to estimate the Lebesgue measure of the spectrum of the Schrödinger operator in terms of geometric parameters of the graph and to point out classes of graphs for which this estimate is sharp;

2) to describe the number and positions of flat bands for Laplacians on specific graphs and to construct a graph, when the number of flat bands is maximal;

3) to analyze the spectrum of the Schrödinger operators on both loop graphs (see definition below) and physical models: face-centered cubic lattice, body-centered cubic lattice and graphene;

4) to obtain stability estimates of bands and gaps in terms of potentials.

The proof of these results is essentially based on a precise form of fiber operators for Laplacians and Schrödinger operators with periodic potentials on periodic graphs, constructed in the paper.

1.1. The definition of 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. The graphs under consideration are embedded into $\mathbb{R}^d$. 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 $(u, v)_e \in \mathcal{E}$. We define the degree $\varkappa_v = \deg v$ of the vertex $v \in V$ 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 (see examples in Figs. 7*a*, 10*a*), 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) *Γ has the periods (a basis) $a_1, \ldots, a_d$ in $\mathbb{R}^d$, such that Γ is invariant under translations through the vectors $a_1, \ldots, a_d$:*

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

In the space $\mathbb{R}^d$ we consider a coordinate system with the origin at some point O and with the basis $a_1, \ldots, a_d$. Below the coordinates of all vertices of Γ will be expressed in this coordinate system. From the definition it follows that a $\mathbb{Z}^d$-periodic graph Γ is invariant under translations through any integer vector m in the basis $a_1, \ldots, a_d$:

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