Schrödinger operators on periodic discrete graphs

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Abstract

We consider Schrödinger operators with periodic potentials on periodic discrete graphs. The spectrum of these operators consists of an absolutely continuous part (which is a union of a finite number of non-degenerated spectral bands) and a finite number of flat bands, i.e., eigenvalues of infinite multiplicity.

We obtain the following results: 1) estimates of the Lebesgue measure of the spectrum in terms of geometric parameters of the graph, 2) spectral bands localization in terms of eigenvalues of Schrödinger operators on a finite subgraph (a fundamental domain) of the periodic graph.

The proof is based on Floquet theory and on the precise representation of fiber Schrödinger operators.

Periodic discrete graphs

Let $\Gamma = (V, \mathcal{E})$ be a connected infinite graph, possibly having loops and multiple edges and embedded into $\mathbb{R}^d$. Here V is the set of its vertices and $\mathcal{E}$ is the set of its unoriented edges.

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

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

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

Examples of periodic graphs

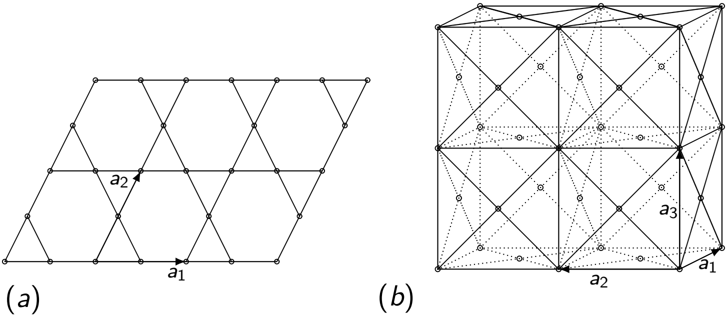


Figure: *a*) Kagome lattice; *b*) Face-centered cubic lattice.

Discrete Laplace operator

Let $\ell^2(V)$ be the Hilbert space of all square summable 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 normalized Laplacian Δ on $\ell^2(V)$ by

$$\big(\Delta f\big)(v) = -\frac{1}{\sqrt{\varkappa_v}} \sum_{(v,u)\in\mathcal{E}} \frac{1}{\sqrt{\varkappa_u}} f(u), \quad v \in V, \quad f \in \ell^2(V), \quad (1)$$

where $\varkappa_v$ is the degree of the vertex v and all loops in the sum (1) are counted twice.

It is known that

$$-1 \in \sigma(\Delta) \subset [-1, 1].$$

Discrete Schrödinger operator

The Schrödinger operator H acts on $\ell^2(V)$ and is defined by

$$H = \Delta + Q,$$

where Δ is the normalized Laplacian,

$$\big(Qf\big)(v) = Q(v)f(v), \quad \forall\, v \in V.$$

The potential Q is real valued and satisfies

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

$a_1, \ldots, a_d$ are the periods of Γ.

Spectrum of Schrödinger operator

In $\mathbb{R}^d$ we consider a coordinate system with the origin at some point O and with the basis $a_1, \ldots, a_d$ (the periods of the graph).

Denote by V_* the set of all vertices of the graph from *the unit cell* $[0,1)^d$:

$$V_* = [0,1)^d \cap V = \{v_1, \ldots, v_\nu\}, \qquad \nu = \# V_* < \infty.$$

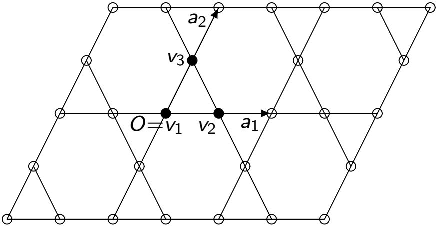


Figure: The unit cell $[0,1)^2$ of the Kagome lattice. The vertices from $V_* = \{v_1, v_2, v_3\}$ are black.

Denote the potential at the vertices of the unit cell by

$$Q(v_n) = q_n, \qquad n \in \mathbb{N}_\nu = \{1, \ldots, \nu\}.$$

Spectrum of Schrödinger operator

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

$$\ell^2(V) = \frac{1}{(2\pi)^d} \int_{\mathbb{T}^d}^{\oplus} \ell^2(V_*)\, d\vartheta, \quad UHU^{-1} = \frac{1}{(2\pi)^d} \int_{\mathbb{T}^d}^{\oplus} H(\vartheta) d\vartheta,$$

$\mathbb{T}^d = \mathbb{R}^d/(2\pi\mathbb{Z})^d$, $\ell^2(V_*) = \mathbb{C}^\nu$ is the fiber space, U is some unitary operator, the Floquet $\nu \times \nu$ matrix $H(\vartheta)$ is given by

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

Each Floquet $\nu \times \nu$ matrix $H(\vartheta)$ has ν eigenvalues labeled by

$$\lambda_1(\vartheta) \leqslant \ldots \leqslant \lambda_\nu(\vartheta), \qquad \vartheta \in \mathbb{T}^d.$$

Spectrum of Schrödinger operator

The real function $\lambda_n(\cdot)$ is continuous on the torus $\mathbb{T}^d$ and creates the spectral band

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

Then the spectrum of H on Γ is given by

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

Note that if $\lambda_n(\cdot) = C_n = \mathrm{const}$ on some set $\mathscr{B} \subset \mathbb{T}^d$ of positive Lebesgue measure, then H on Γ has the eigenvalue C_n with infinite multiplicity (*flat band*). Thus, the spectrum of H on Γ has the form

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

Here $\sigma_{ac}(H)$ is the absolutely continuous spectrum (a union of non-degenerated intervals), and $\sigma_{fb}(H) = \{\mu_1, \ldots, \mu_r\}$, $r < \nu$, is the set of all flat bands. An open interval between two neighboring non-degenerated spectral bands is called a *gap*.

Example (stanene)

The Floquet 4×4 matrix $\Delta(\vartheta)$ is given by

$$\Delta(\vartheta) = -\begin{pmatrix} 0 & \frac{1}{2} & \frac{b(\vartheta)}{4} & 0 \\ \frac{1}{2} & 0 & 0 & 0 \\ \frac{\overline{b}(\vartheta)}{4} & 0 & 0 & \frac{1}{2} \\ 0 & 0 & \frac{1}{2} & 0 \end{pmatrix}, \quad b(\vartheta) = 1 + e^{i\vartheta_1} + e^{i\vartheta_2}.$$

The characteristic equation for the matrix $\Delta(\vartheta)$

$$\lambda^4 - \lambda^2 \left(\frac{1}{2} + \frac{|b(\vartheta)|^2}{16} \right) + \frac{1}{16} = 0.$$

The eigenvalues of each matrix $\Delta(\vartheta)$ are given by

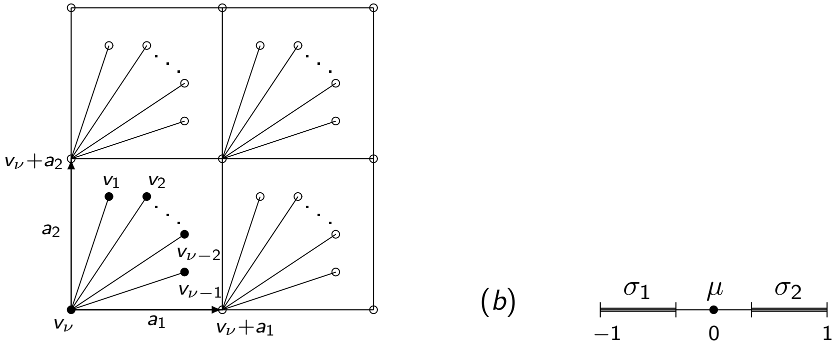
$$\lambda_{1,2,3,4}(\vartheta) = \pm \frac{|b(\vartheta)|}{8} \pm \frac{\sqrt{|b(\vartheta)|^2 + 16}}{8}.$$

The spectrum of the Laplacian on Γ has the form

$$\sigma(\Delta) = \sigma_{ac}(\Delta) = [-1; -0.5] \cup [-0.5; -0.25] \cup [0.25; 0.5] \cup [0.5; 1].$$

Example (d-dimensional lattice with pendant edges)

(a) (b)



The spectrum of the Laplacian Δ

$$\sigma(\Delta) = \sigma_{ac}(\Delta) \cup \sigma_{fb}(\Delta),\ \sigma_{fb}(\Delta) = \{0\},\ \sigma_{ac}(\Delta) = \sigma_1(\Delta) \cup \sigma_2(\Delta),$$

$$\sigma_1(\Delta) = [-1, -1 + \tfrac{2d}{\xi}], \qquad \sigma_2(\Delta) = [1 - \tfrac{2d}{\xi}, 1], \qquad \xi = \nu - 1 + 2d.$$

Adding a *generic* potential ($q_j \neq q_k$ for all $j, k \in \mathbb{N}_\nu$, $j \neq k$) destroys the flat bands.

What is the maximum number of flat bands?

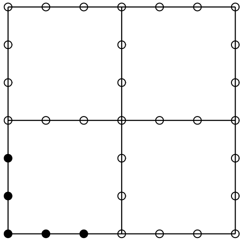


Figure: Graph Γ obtained by adding $N = 2$ vertices on each edge of the square lattice.

The spectrum of the Laplacian on Γ has the form

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

where $\sigma_{ac}(\Delta) = [-1, 1]$ is the absolutely continuous part and the set of all flat bands has the form

$$\sigma_{fb}(\Delta) = \Big\{ \cos \frac{\pi n}{N+1} \ : \ n = 1, \ldots, N \Big\}.$$

Bridges

Recall that the set of all vertices of the graph from *the unit cell* $[0,1)^d$ is denoted by V_*:

$$V_* = [0,1)^d \cap V = \{v_1, \ldots, v_\nu\}, \qquad \nu = \#V_* < \infty.$$

Bridges of the unit cell are the edges of Γ connecting the vertices from V_* (black points) with the vertices from $V \setminus V_*$ (white points).

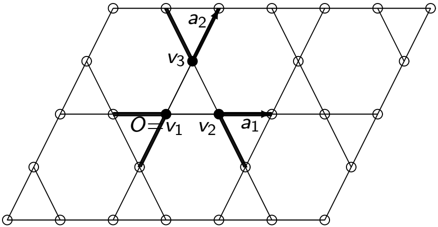


Figure: The unit cell $[0,1)^2$ of the Kagome lattice. The vertices from $V_* = \{v_1, v_2, v_3\}$ are black and the bridges are bold.

Theorem 1. *The Lebesgue measure $|\sigma(H)|$ of the spectrum of the Schrödinger operator $H = \Delta + Q$ satisfies*

$$|\sigma(H)| \leqslant \sum_{n=1}^{\nu} |\sigma_n(H)| \leqslant 2\beta\,, \qquad \beta = \sum_{n=1}^{\nu} \frac{\beta_n}{\varkappa_n}\,, \tag{2}$$

β_n is the bridge degree (the number of bridges incident to v_n) and $\varkappa_n$ is the degree of $v_n \in V_*$. Moreover, if in the spectrum $\sigma(H)$ there exist s spectral gaps $\gamma_1(H), \dots, \gamma_s(H)$, then

$$\sum_{n=1}^{s} |\gamma_n(H)| \geqslant C - 2\beta, \quad C = \max\{\hat{\lambda} - q_\bullet + 1\,,\, q_\bullet - 2\},$$

$q_\bullet = \max_n q_n - \min_n q_n$; $\hat{\lambda}$ is the upper point of the spectrum of Δ.

Remark. 1) In the case $H = \Delta$ the estimate (2) is not trivial iff $\beta < 1$. This condition holds when the number of bridges at each vertex $v \in V_*$ is sufficiently small compared to the degree of the vertex.

2) For some classes of graphs the estimate (2) becomes an identity.

How does it work?

$$|\sigma(\Delta)| \leqslant 2\beta, \qquad \beta = \sum_{n=1}^{\nu} \frac{\beta_n}{\varkappa_n}\,. \tag{3}$$

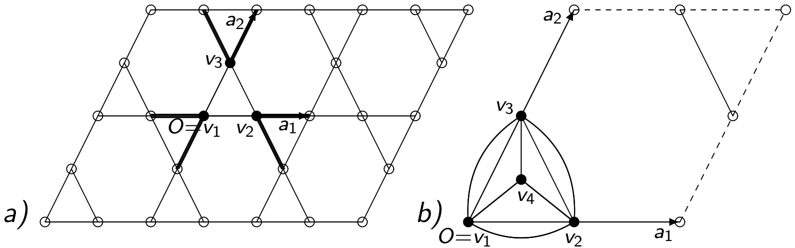


Figure: *a)* The Kagome lattice; *b)* the unit cell of a new graph, obtained from the Kagome lattice by adding vertices and edges.

For the Kagome lattice $\beta = 3 \cdot \frac{2}{4} = \frac{3}{2} > 1.$ The estimate (3) is trivial.

For the new graph $\beta = 3 \cdot \frac{2}{7} = \frac{6}{7} < 1.$ The estimate (3) gives $|\sigma(\Delta)| \leqslant \frac{12}{7} < 2.$

Example (decorations of d-dimensional lattice)

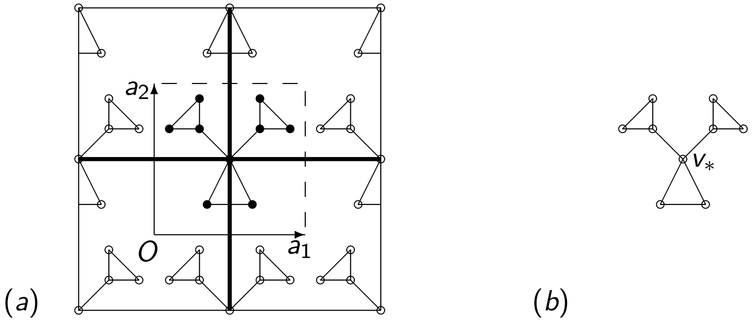


Figure: a) Decorated square lattice; b) finite graph.

For a decorated d-dimensional lattice

$$|\sigma(H)| = 2\beta, \qquad \beta = \sum_{n=1}^{\nu} \frac{\beta_n}{\varkappa_n} = \frac{2d}{2d + \varkappa_*}.$$

The Lebesgue measure $|\sigma(H)|$ of the spectrum of $H = \Delta + Q$ **does not depend on** the potential Q.

For the decorated square lattice $\beta = \frac{4}{8}$ and we have $|\sigma(H)| = 1$.

Localization of spectral bands

Lledó and Post (2008) obtained the spectral band localization (*eigenvalue bracketing*) for the Laplacians on metric graphs. Via an explicit correspondence of the metric and discrete graph spectrum they carry over these estimates from the metric graph Laplacian to the discrete case. Finally, they write

"*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.*"

Lledó, F.; Post, O. Eigenvalue bracketing for discrete and metric graphs, J. Math. Anal. Appl. 348 (2008), 806–833.

Fundamental domain of periodic graph

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* $V_1 \supset V_*$; V_* *is the set of all vertices of the graph from the unit cell* $[0, 1)^d$;

2) Γ_1 *does not contain any* $\mathbb{Z}^d$*-equivalent edges;*

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

The fundamental domain Γ_1 is not uniquely defined and we fix one of them.

Example of fundamental domain

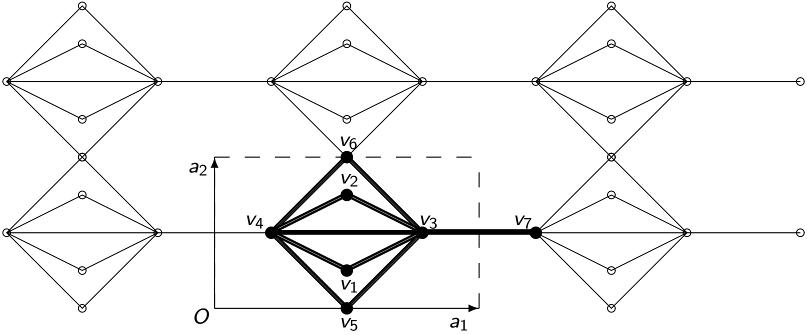


Figure: Periodic graph Γ and one of its fundamental domain Γ_1 (the vertices and the edges of Γ_1 are bold). The set of all vertices of the unit cell $V_* = \{v_1, \ldots, v_5\}$.

We define the set V_0 of *all inner vertices* of $\Gamma_1 = (V_1, \mathcal{E}_1)$ by

$$V_0 = \{v \in V_1 : \varkappa_v = \varkappa_v^1\},$$

where $\varkappa_v^1$ is the degree of the vertex $v \in V_1$ on the graph Γ_1.

We define a *boundary* ∂V_1 of Γ_1 by the identity:

$$\partial V_1 = V_1 \setminus V_0.$$

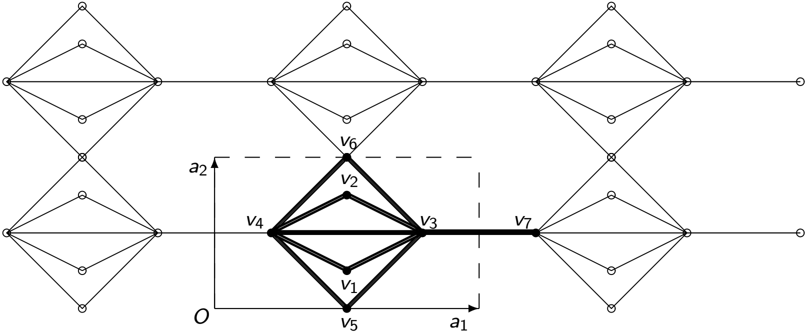


Figure: Periodic graph Γ and its fundamental domain Γ_1 (the vertices and the edges of Γ_1 are bold). The set of inner vertices $V_0 = \{v_1, v_2, v_3\}$ and the boundary $\partial V_1 = \{v_4, v_5, v_6, v_7\}$.

On the finite graph $\Gamma_1 = (V_1, \mathcal{E}_1)$ we define two self-adjoint operators H_1 and H_0:

1) The operator H_1 on $\ell^2(V_1)$ is the discrete Schrödinger operator on the graph Γ_1.

2) The Dirichlet operator H_0 on $f \in \ell^2(V_1)$ is defined by

$$H_0 f = H_1 f, \quad \text{where} \quad f|_{\partial V_1} = 0.$$

Let $\nu_\phi = |V_\phi|$ be the number of vertices in V_ϕ, $\phi = 0, 1$.

Denote by

$$\lambda_1^\phi \leqslant \lambda_2^\phi \leqslant \ldots \leqslant \lambda_{\nu_\phi}^\phi$$

the eigenvalues of the operators H_ϕ, $\phi = 0, 1$, counted according to multiplicity.

We rewrite the sequence $q_1, \ldots, q_\nu$ in nondecreasing order

$$q_1^\bullet \leqslant q_2^\bullet \leqslant \ldots \leqslant q_\nu^\bullet.$$

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 2. *Each spectral band $\sigma_n(H)$ of the discrete Schrödinger operator $H = \Delta + Q$ on the periodic graph Γ satisfies*

$$\sigma_n(H) \subset J_n \cap K_n, \qquad n \in \mathbb{N}_\nu,$$

where the intervals J_n, K_n are given by

$$J_n = \begin{cases} [\lambda_n^1, \lambda_n^0], & n = 1, \ldots, \nu_0 \\ [\lambda_n^1, q_n^\bullet + 1], & n = \nu_0 + 1, \ldots, \nu, \end{cases}$$

$$K_n = \begin{cases} [q_n^\bullet - 1, \lambda_{n+\nu_1-\nu}^1], & n = 1, \ldots, \nu - \nu_0 \\ [\lambda_{n-\nu+\nu_0}^0, \lambda_{n+\nu_1-\nu}^1], & n = \nu - \nu_0 + 1, \ldots, \nu \end{cases}.$$

Remark. 1) Theorem 2 estimates the position of the spectral bands in terms of eigenvalues of the operators H_1 and H_0 on the finite graph Γ_1.

2) In some cases Theorem 2 allows to detect the existence of gaps and flat bands in the spectrum of the Schrödinger operator H.

3) Lledó and Post (2008) obtained the estimate $\sigma_n(\Delta) \subset J_n$ for the Laplacian Δ.

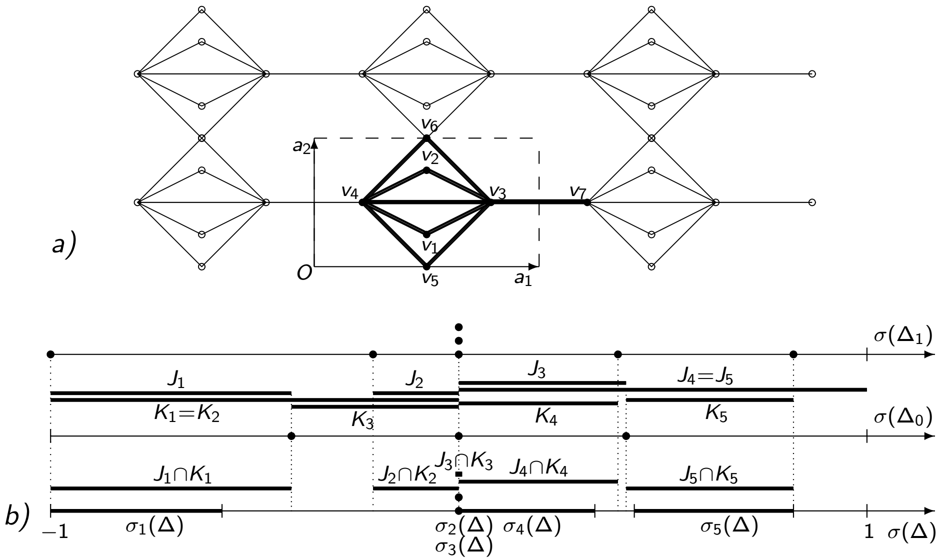


Figure: *a)* A periodic graph Γ and its finite graph Γ_1, the vertices and the edges of Γ_1 are bold; *b)* Eigenvalues of the operators Δ_1 and Δ_0, the intervals J_n and K_n, $n \in \mathbb{N}_5$, and their intersections, the spectrum of the Laplacian Δ.

The similar results can be formulated for the combinatorial Laplacians

$$\big(\Delta_* f\big)(v) = \sum_{(v,u)\in\mathcal{E}} \big(f(v) - f(u)\big), \quad v \in V, \quad f \in \ell^2(V),$$

and for the Schrödinger operators $H_* = \Delta_* + Q$.

Thank you for attention!