Spectra of periodic quantum graphs

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1 Periodic graphs

2 Floquet Theory

3 Floquet Theory and Periodic Graphs

4 Flat Bands

5 Quantum graphs
- Metric Graphs
- Quantum Graphs
- $\mathbb{Z}^2$-periodic Quantum Graphs

6 Spectra of $\mathbb{Z}^2$-periodic Quantum graphs
- The Secular Matrix
- Example for square lattice

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3 Floquet Theory and Periodic Graphs

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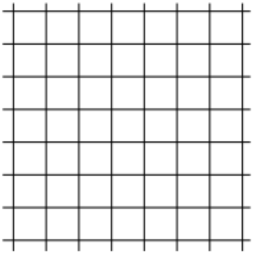
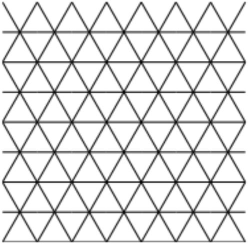
Periodic graph

Periodic graphs are infinite graphs with a repetitive structure. They have a finite description (the *fundamental domain*) given by a connected graph with weights associated with the edges.

Examples



(4^4)



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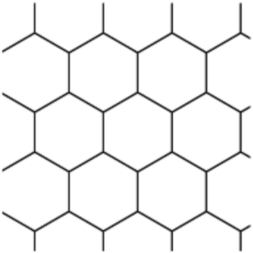

(6^3)

Periodic graph

Locally finite $\mathbb{Z}^d$-periodic graphs $G = (V, E)$, with the vertex set V and edge E, are graphs satisfying the following conditions:

1. The degree of each vertex is finite;
2. There exists a basis $w_1, \ldots, w_d$ in $\mathbb{R}^d$ (the so-called periods of G) such that G is invariant under translations through the vectors $w_1, \ldots, w_d$:

$$G + w_s = G, \forall s \in \mathbb{N}_d = \{1, \ldots, d\}.$$

Fundamental domain

Periodic graph can be constructed by repeating a smaller graph called a **fundamental domain**.

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Periodic graph can be constructed by repeating a smaller graph called a **fundamental domain**.
We give a definition for $d = 2$:

Definition

There exists a finite part Q of G such that

* The union of all $\mathbb{Z}^2$-shifts of Q covers the whole G:

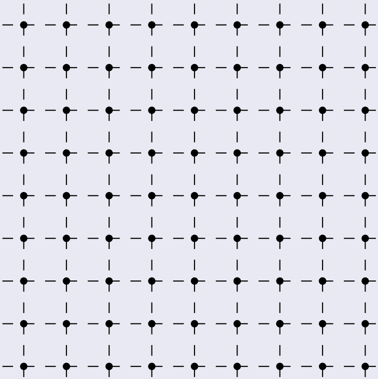
$$\bigcup_{k \in \mathbb{Z}^2} Q + k = G.$$

A finite subset Q with this property is a **fundamental domain** for the action of $\mathbb{Z}^2$ on G.

Note that the set of vertices is $V = Q \times \mathbb{Z}^2$.

How to use the periodicity

The square lattice that covers the whole plane



How to use the periodicity

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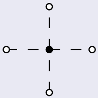

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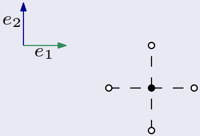
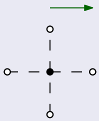


How to use the periodicity

... and by shifting via $\mathbb{Z}^2$



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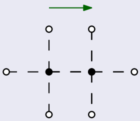

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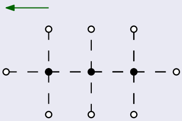

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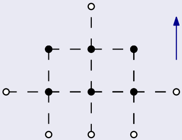

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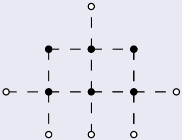

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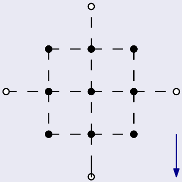

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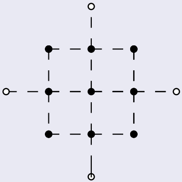

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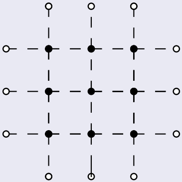

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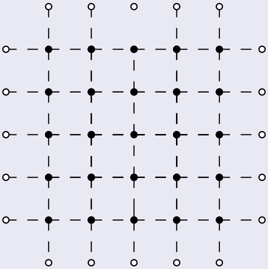

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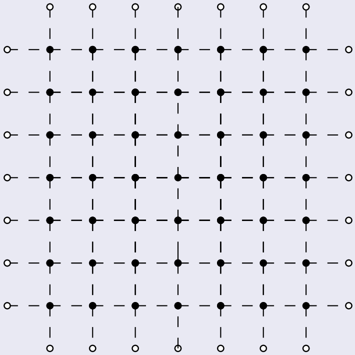

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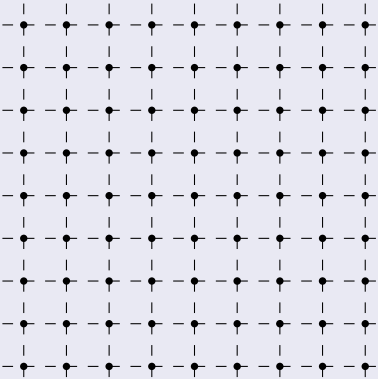
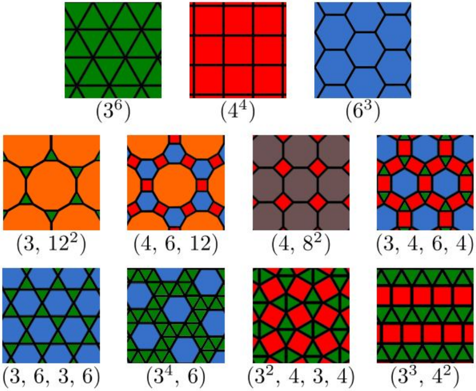


Archimedean tiling

Examples of periodic graphs are given by Archimedean tilings. They were systematically investigated in 1619 by Johannes Kepler: he identified all 11 Archimedean tilings, namely with vertices of type (4^4), (3^6), (6^3), $(3.6)^2$, (3.12^2), (4.8^2), $(3^3.4^2)$, $(3^2.4.3.4)$, $(3.4.6.4)$, $(3^4.6)$ and $(4.6.12)$.



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Floquet transform

- Floquet theory is the main tool that allows to reduce periodic operators to finite simpler operators.
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Floquet transform on periodic graphs

Let G be a $\mathbb{Z}^2$-periodic graph.
Let $\mathbb{T}^2 = \mathbb{R}^2/2\pi\mathbb{Z}^2$ be the 2-dimensional flat torus.
We define the Floquet transform, denoted by $\mathcal{U}$, as the partial Fourier transform in the second component.

$$\begin{aligned} \mathcal{U} : \ell^2(Q \times \mathbb{Z}^2) &\to L^2(Q \times \mathbb{T}^2) \\ f &\mapsto \mathcal{U}(f)(v,\theta) = \sum_{k\in\mathbb{Z}^2} f(v+k)e^{-i\theta k}. \end{aligned}$$

Periodic Laplacian

Definition

For every $\theta \in \mathbb{T}^2$, we have the $|Q|$-dimensional Hilbert space $\ell^2(V)_\theta$ defined as follow :

$$\ell^2(V)_\theta := \{\hat{f} : V \to \mathbb{C}, \hat{f}(v+k) = e^{ik\theta}\hat{f}(v) \text{ for all } k \in \mathbb{Z}^2\}.$$

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We consider the periodic graph $G = (V, E)$. Let Δ be the Laplacian on G. The θ-pseudoperiodic Laplacian $\Delta_\theta : \ell^2(V)_\theta \to \ell^2(V)_\theta$ on G is defined as

$$(\Delta_\theta f)(v) = f(v) - \frac{1}{\deg(v)} \sum_{w \sim v} f(w).$$

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Since $\ell^2(V)_\theta$ is a $|Q|$-dimensional vector space due to quasiperiodicity, the operator Δ_θ can be viewed as a hermitian matrix with order $|Q|$. This operator is called **Floquet Matrix**.

Floquet magic

For $\theta \in \mathbb{T}^2$ and $p \in V$, we have

$$(\mathcal{U}\Delta f)_p(\theta) = [\Delta_\theta(\mathcal{U}f)(\theta)]_p \qquad \text{for all } f \in \ell^2(V).$$

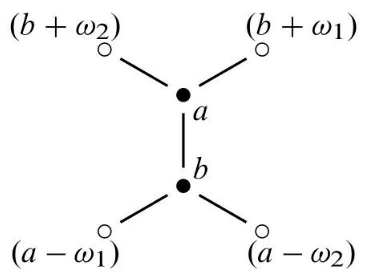
Theorem

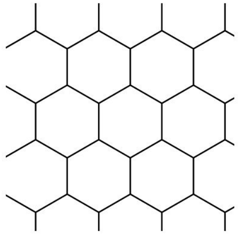
The spectrum $\sigma(\Delta)$ of the operator Δ in $\ell^2(V)$ equals the union of the spectra $\sigma(\Delta_\theta)$ of the operator Δ_θ,

$$\sigma(\Delta) = \bigcup_{\theta \in \mathbb{T}^2} \sigma(\Delta_\theta).$$

The 6^3 (honeycomb) tiling

Fundamental domain of the (6^3)





(6^3)

The 6^3 (honeycomb) tiling

A fundamental domain of the honeycomb tiling consists of two points. We have the Floquet matrix

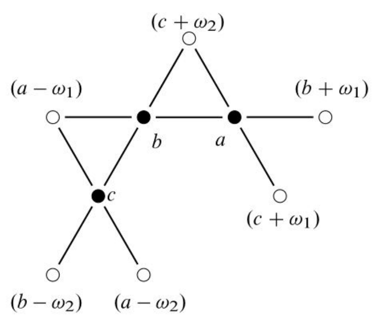
$$\Delta^\theta = \begin{pmatrix} 1 & -\frac{1}{3}(1+e^{i\theta_1}+e^{i\theta_2}) \\ -\frac{1}{3}(1+e^{-i\theta_1}+e^{-i\theta_2}) & 1 \end{pmatrix}$$

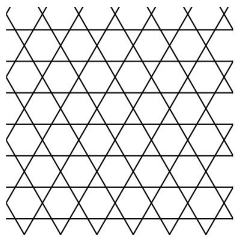
with eigenvalues

$$\begin{cases} \lambda^\theta_{(6^3),1} = 1 - \frac{1}{3}\sqrt{2\cos\theta_1 + 2\cos\theta_2 + 2\cos(\theta_1-\theta_2)+3}, \\ \lambda^\theta_{(6^3),2} = 1 + \frac{1}{3}\sqrt{2\cos\theta_1 + 2\cos\theta_2 + 2\cos(\theta_1-\theta_2)+3}. \end{cases}$$

The $(3.6)^2$ tiling (the kagome lattice)

Fundamental domain of the $(3.6)^2$





$(3.6)^2$

The $(3.6)^2$ tiling (the kagome lattice)

A fundamental domain of the kagome lattice consists of three points, with the Floquet matrix

$$\Delta_\theta = I - \frac{1}{4}\begin{pmatrix} 0 & (1+e^{i\theta_1}) & (e^{i\theta_1}+e^{i\theta_2}) \\ (1+e^{-i\theta_1}) & 0 & (1+e^{i\theta_2}) \\ (e^{-i\theta_1}+e^{-i\theta_2}) & (1+e^{-i\theta_2}) & 0 \end{pmatrix}$$

and with eigenvalues

$$\begin{cases} \lambda^\theta_{(3.6)^2,1} = \frac{3-\sqrt{3+2(\cos(\theta_1)+\cos(\theta_2)+\cos(\theta_1-\theta_2))}}{4}, \\ \lambda^\theta_{(3.6)^2,2} = \frac{3+\sqrt{3+2(\cos(\theta_1)+\cos(\theta_2)+\cos(\theta_1-\theta_2))}}{4}, \\ \lambda^\theta_{(3.6)^2,3} = \frac{3}{2} \end{cases}$$

Table of contents

1. Periodic graphs
2. Floquet Theory
3. Floquet Theory and Periodic Graphs
4. Flat Bands
5. Quantum graphs
6. Spectra of $\mathbb{Z}^2$-periodic Quantum graphs

Floquet Theory and Periodic Graphs

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Then it is possible to use Floquet Theory to study the spectrum of the operator Δ.

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Flat Bands

Since the eigenvalues of Δ_θ depends continously on θ

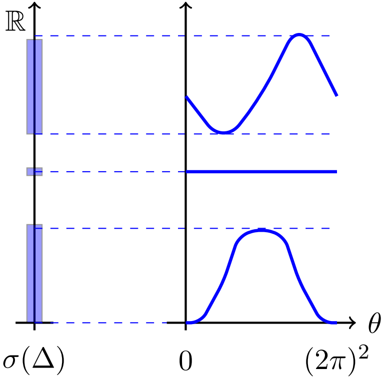
$$\sigma(\Delta) = \bigcup_{\theta \in \mathbb{T}^2} \sigma(\Delta_\theta)$$

consists of intervals. If

$$\lambda_0 \in \bigcap_{\theta \in \mathbb{T}^2} \sigma(\Delta_\theta),$$

then it is called a **flat band**. It can be seen that flat bands are eigenvalues with infinite multiplicity of Δ.

Flat Bands



$\leftarrow$ Flat band

Eigenvalues of Δ

Flat bands and eigenvectors of finite support

Theorem

If Δ has a flat band then it has a corresponding eigenvector of finite support and we know how to find such an eigenfunction.

The proof uses two lemmas.

First Lemma

Let G has a finite fundamental domain Q and let λ_0 be a flat band. Then there is a θ - dependent family of eigenfunctions $(f(\theta))_{\theta\in\mathbb{T}^2}$ of Δ_θ with eigenvalue λ_0, where the p-th entry is of the form

$$f_p(\theta) = \sum_{m\in\Lambda_p} \alpha_p(m) e^{im\cdot\theta},$$

where $\Lambda_p \subset \mathbb{Z}^2$ is some finite set. So, the $f_p(\theta)$ are trigonometric polynomials in $(\theta_i)_{i=1,2}$ with frequencies in $\mathbb{Z}^2$.

Proof of First Lemma, step 1

Step 1.

Claim. For almost every $\theta \in \mathbb{T}^2$, λ_0 has the same multiplicity.

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Let

$$m = \min_\theta \{\text{multiplicity of } \lambda_0 \text{ of } \Delta_\theta\}.$$

Consider the characteristic polynomial of Δ_θ

$$\det(\Delta_\theta - \lambda Id) = (\lambda - \lambda_0)^m g(\theta, \lambda),$$

where the map

$$\theta \mapsto g(\theta, \lambda) \quad \text{is analytic.}$$

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Assume that

$$g(\theta, \lambda_0) = 0 \quad \text{for} \quad \theta \in S \subset \mathbb{T}^2,$$

where S is a Lebesgue-measurable set of positive measure, so by analyticity it must be

Proof of First Lemma, step 1

So we can rewrite the function $g(\theta, \lambda)$ as following

$$g(\theta, \lambda) = (\lambda - \lambda_0)\tilde{g}(\theta, \lambda)$$

and we obtain

$$\begin{aligned} \det(\Delta_\theta - \lambda Id) &= (\lambda - \lambda_0)^m g(\theta, \lambda) \\ &= (\lambda - \lambda_0)^{m+1}\tilde{g}(\theta, \lambda). \end{aligned}$$

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So we get a contradiction because we supposed that m was the minimum, so the assumption is wrong, hence $g(\theta, \lambda_0) \neq 0$ and m is the multiplicity that we were looking for.

Proof of First Lemma, step 2

Step 2.

Claim. $(\Delta_\theta - \lambda_0)g(\theta, \Delta_\theta) = 0.$

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$$(\Delta_\theta - \lambda_0)^m g(\theta, \Delta_\theta) = 0.$$

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Let $n = |Q|$. Take

$$v_{0,1}(\theta), \dots, v_{0,m}(\theta) \quad \text{eigenvectors of } \lambda_0,$$

$$v_{m+1}(\theta), \dots, v_{n-1}(\theta) \quad \text{eigenvectors of the others eigenvalues.}$$

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We want to prove

$$(\Delta_\theta - \lambda_0)g(\theta, \Delta_\theta)v_k(\theta) = 0, \quad k = m, \ldots, n-1.$$

Indeed, we have

$$g(\theta, \Delta_\theta)v_k(\theta) = g(\theta, \lambda_k(\theta)v_k(\theta) = 0 \quad \Longrightarrow \quad (\Delta_\theta - \lambda_0)g(\theta, \Delta_\theta)v_k(\theta) = 0.$$

Proof of First Lemma, step 2

We also want to prove

$$(\Delta_\theta - \lambda_0) g(\theta, \Delta_\theta) v_{0,k}(\theta) = 0.$$

By commutative property we have

$$g(\theta, \Delta_\theta)(\Delta_\theta - \lambda_0) v_k(\theta) = 0,$$

and

$$(\Delta_\theta - \lambda_0) v_k(\theta) = 0.$$

So we proved Claim 2.

Proof of First Lemma, step 3

Step 3. (Construction of a eigenfunction)

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The matrix $g(\theta, \Delta_\theta)$ is not zero. Indeed, by step 1, we know that $g(\theta, \lambda_0) \neq 0$. Hence,

$$\{0\} \neq g(\theta, \sigma(\lambda_\theta)) = \sigma(g(\theta, \Delta_\theta)) \implies g(\theta, \Delta_\theta) \neq 0,$$

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Finally, we define the eigenfunction $f(\theta)$.

We expand $g(\theta, \Delta_\theta)$ in column form

$$g(\theta, \Delta_\theta) = [g_1(\theta, \Delta_\theta), \ldots, g_n(\theta, \Delta_\theta)].$$

Proof of First Lemma, step 3

Then

$$(\Delta_\theta - \lambda_0)[g_1(\theta, \Delta_\theta), \ldots, g_n(\theta, \Delta_\theta)] = 0,$$

hence

$$[(\Delta_\theta - \lambda_0) g_1(\theta, \Delta_\theta), \ldots, (\Delta_\theta - \lambda_0) g_n(\theta, \Delta_\theta)] = 0,$$

and there exists at least one index i such that

$$(\Delta_\theta - \lambda_0) g_i(\theta, \Delta_\theta) = 0,$$

and

$$0 \neq g_i(\theta, \Delta_\theta).$$

And this $g_i(\theta, \Delta_\theta)$ is the eigenfunction $f(\theta)$ whose entries $f_i(\theta)$ are trigonometric polynomials with integer-valued frequencies in θ.

Second Lemma

If Δ_θ has an eigenvector $f(\theta)$ with entries

$$f_p(\theta) = \sum_{m \in \Lambda_p} \alpha_p(m) e^{im\cdot\theta},$$

then

$$\phi_p(k) = \begin{cases} \alpha_p(k), & \text{if} \quad k \in \Lambda_p, \\ 0, & \text{otherwise}, \end{cases}$$

are entries of an eigenvector ϕ of Δ.

In particular, the constructed eigenvector has finite support.

This lemma is the first part of Lemma 2.6 in [Sabri, Youssef, 2023]

Proof Second Lemma

Let

$$\phi_p(k) = \int_{\mathbb{T}^2} f_p(\theta) e^{ik\cdot\theta}\, d\theta$$

be the preimage of $f_p(\theta)$ under the operator $\mathcal{U}$.

Then

$$(\mathcal{U}\Delta\phi)(\theta) = \Delta_\theta(\mathcal{U}\phi)(\theta) = \lambda(\mathcal{U}\phi)(\theta)$$

so ϕ is an eigenvector of Δ since $\mathcal{U}$ is unitary.

$$\phi_p(k) = \int_{\mathbb{T}^2} f_p(\theta) e^{ik\cdot\theta}\, d\theta = \alpha_p(m) \int_{\mathbb{T}^2} e^{i(k-m)\cdot\theta}\, d\theta = \alpha_p(m)\delta_{k,m}.$$

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Then we have

$$\text{if} \quad m = k \Rightarrow k \in \Lambda_p \Rightarrow \phi_p = \alpha_p(k)$$
$$\text{if} \quad m \neq k \Rightarrow k \notin \Lambda_p \Rightarrow \phi_p = 0$$

so we get the claim.

Table of Contents

1. Periodic graphs
2. Floquet Theory
3. Floquet Theory and Periodic Graphs
4. Flat Bands
5. Quantum graphs
   - Metric Graphs
   - Quantum Graphs
   - $\mathbb{Z}^2$-periodic Quantum Graphs
6. Spectra of $\mathbb{Z}^2$-periodic Quantum graphs
   - The Secular Matrix
   - Example for square lattice

Metric graphs

Metric graphs - a vague definition

A ***metric graph*** is made up of intervals $[0, L_i]$ that are *glued* together at the boundary points.

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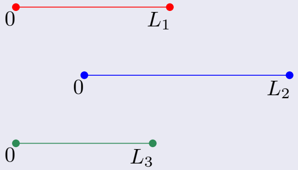

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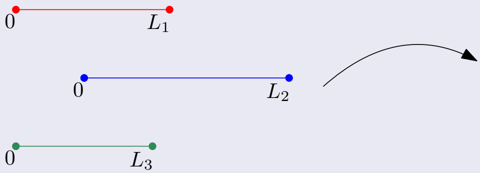

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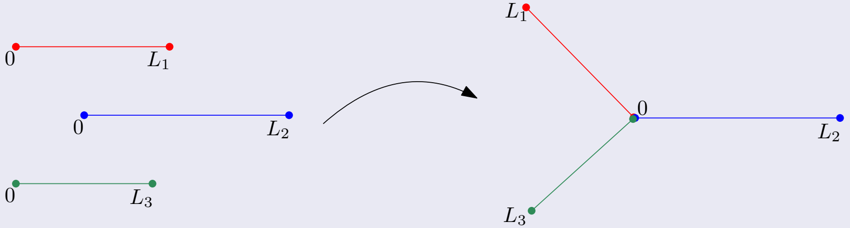

Metric Graphs

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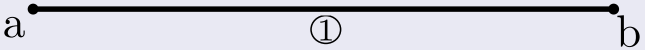
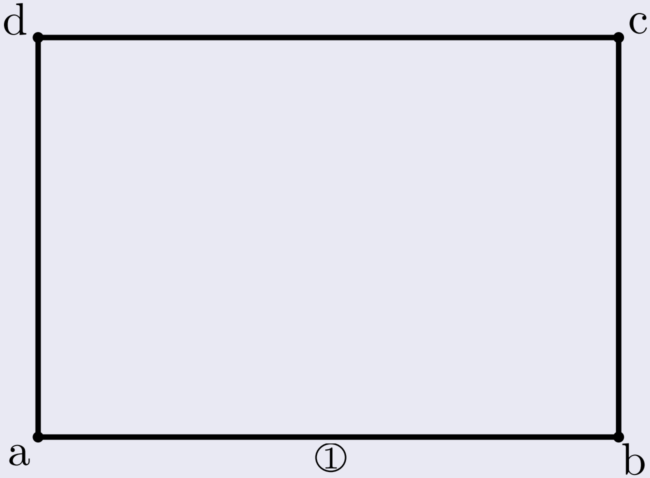



a
①
b

Metric Graphs



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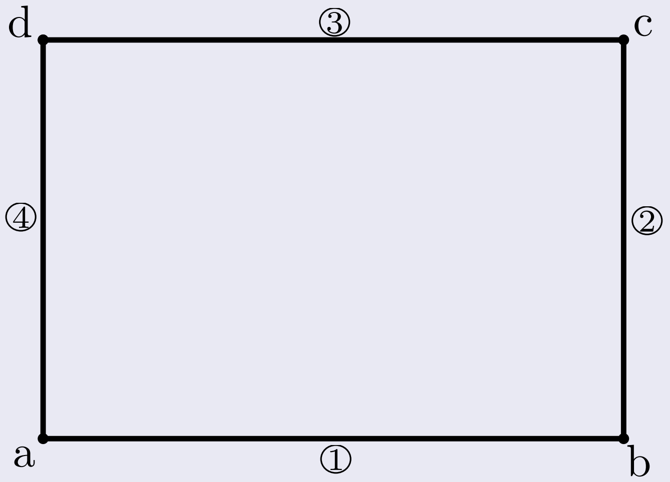

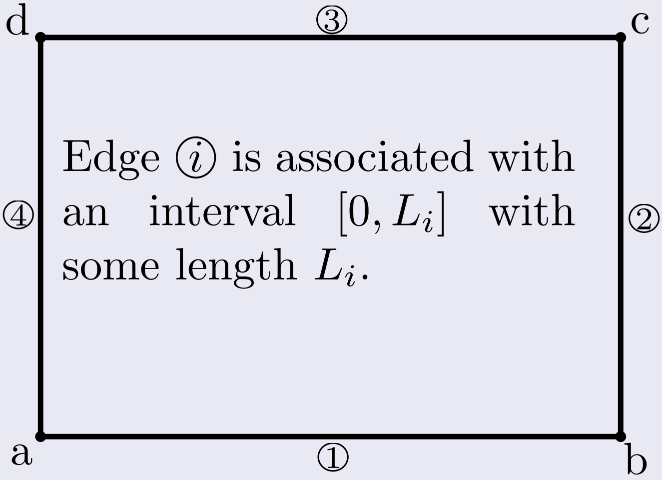

Edge ⓘ is associated with an interval $[0, L_i]$ with some length L_i.

Metric Graphs - an (almost) formal definition

Let $G = (\mathcal{V}, \mathcal{E}, L, o)$ be a locally finite weighted graph with orientation, i.e.

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The graph G is said to be a associated to a ***metric graph*** $\mathcal{G}$ if each edge $e \in \mathcal{E}$ is identified with the finite interval $[0, L_e]$ as well as the initial and terminal point of $o(e)$ with 0 and L_e respectively.

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By a slight abuse of notation we also write e to denote the associated interval $[0, L_e]$.

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Every ***metric graph*** becomes canonically a *measure space* with the Lebesgue measure on the intervals $[0, L_e]$.

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i.e. $f \in L^2(\mathcal{G})$ *if and only if* there are $f_e \in L^2(e)$ such that

$$f = (f_e)_{e \in \mathcal{E}} \qquad \text{and} \qquad \sum_{e \in \mathcal{E}} \|f_e\|^2_{L^2(e)} < \infty.$$

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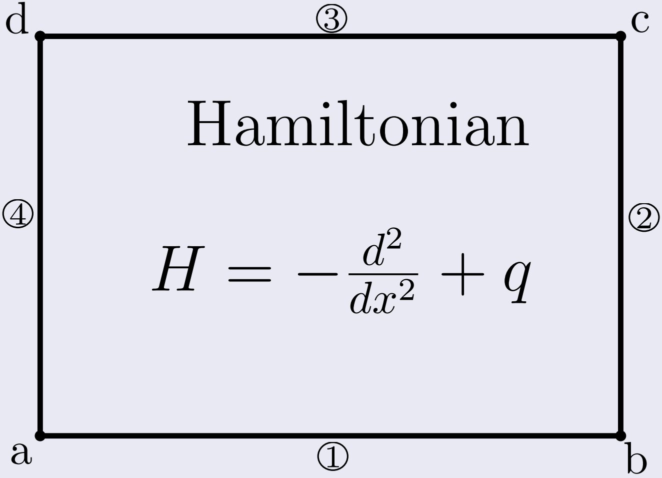
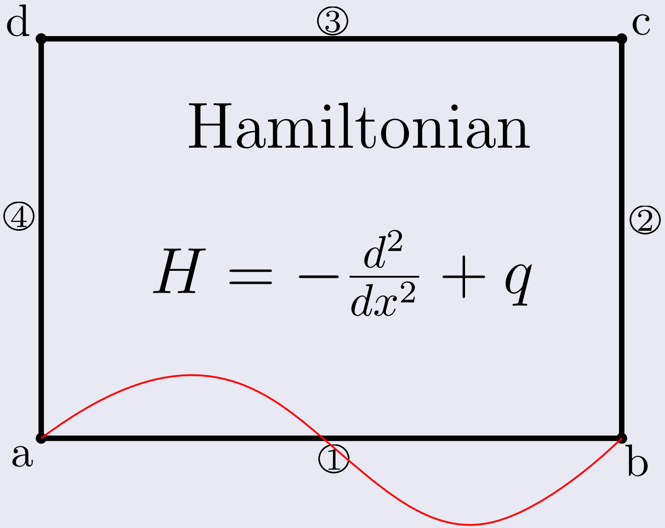
in particular, the inner product on $L^2(\mathcal{G})$, is given by

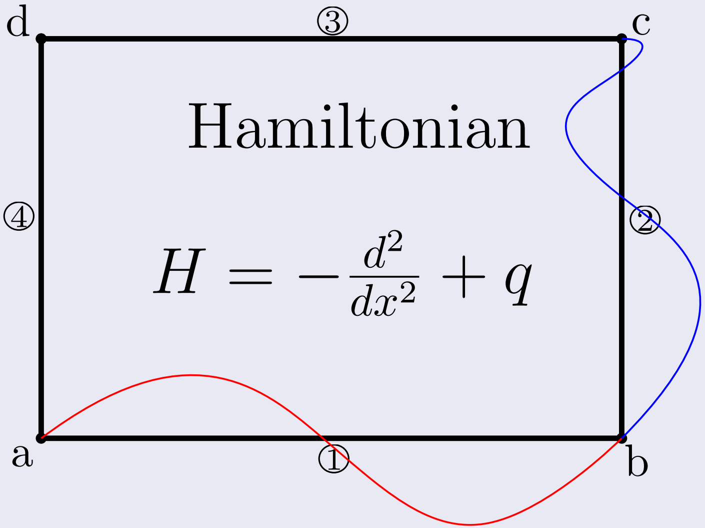
$$\langle f, g \rangle = \int_{\mathcal{G}} \overline{f}\, g dx = \sum_{e \in \mathcal{E}} \int_{[0,L_e]} \overline{f_e}\, g_e dx \quad \text{for all } f, g \in L^2(\mathcal{G}).$$

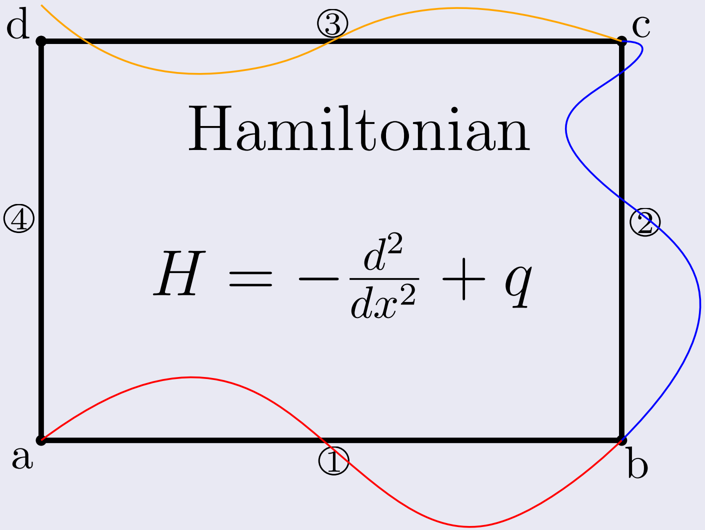


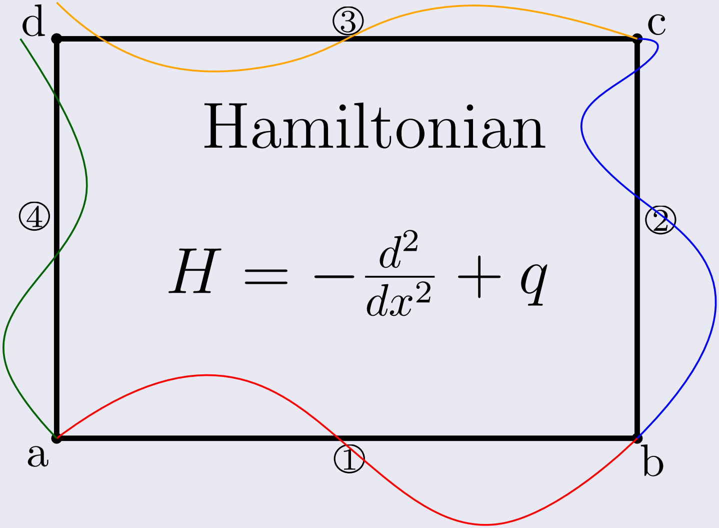
$$H = -\frac{d^2}{dx^2} + q$$

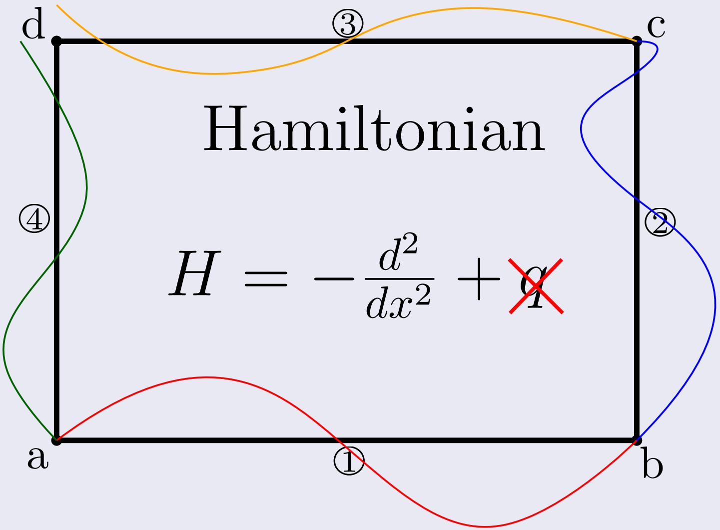
Quantum Graphs

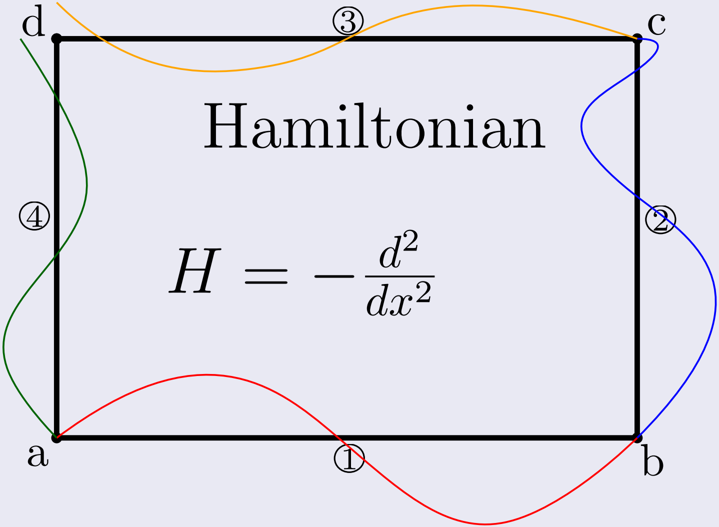


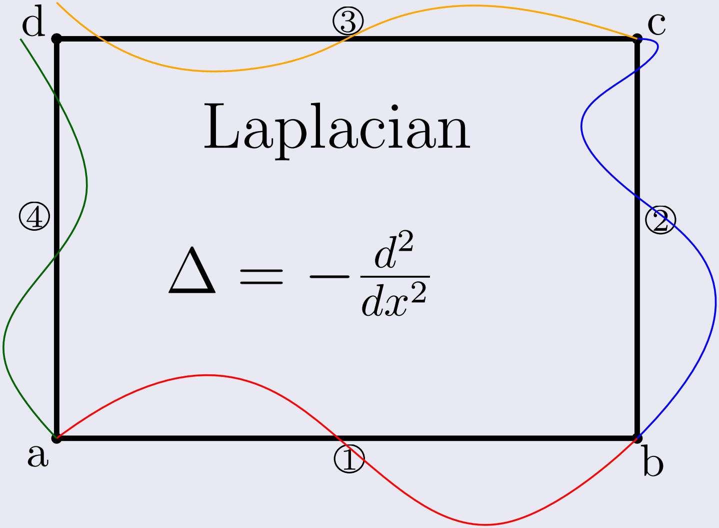

d
③
c
Hamiltonian
④
②
$H = -\frac{d^2}{dx^2} + q$
a
①
b

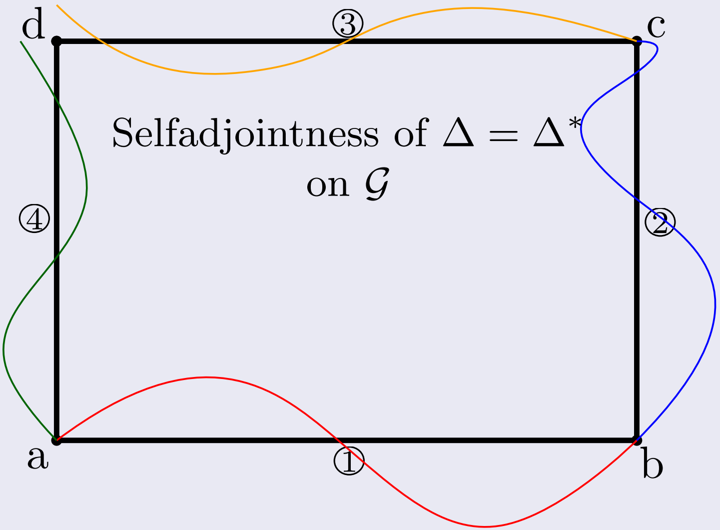

d
③
c
Hamiltonian
④
②
$H = -\frac{d^2}{dx^2} + q$
a
①
b

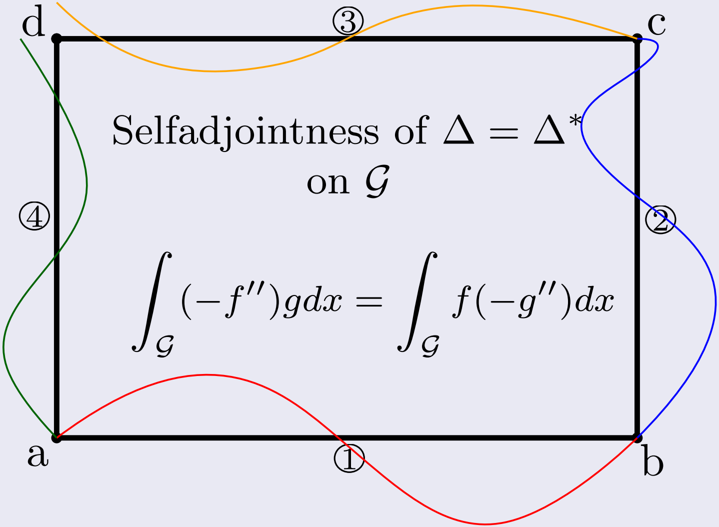

d
③
c
Hamiltonian
④
②
$H = -\frac{d^2}{dx^2} + q$
a
①
b


d
③
c
Hamiltonian
④
②
$H = -\frac{d^2}{dx^2} + \cancel{q}$
a
①
b


d
③
c
Hamiltonian
④
②
$H = -\frac{d^2}{dx^2}$
a
①
b


d
③
c
Laplacian
④
②
$\Delta = -\frac{d^2}{dx^2}$
a
①
b


d
③
c
Selfadjointness of $\Delta = \Delta^*$
on $\mathcal{G}$
④
②
a
①
b

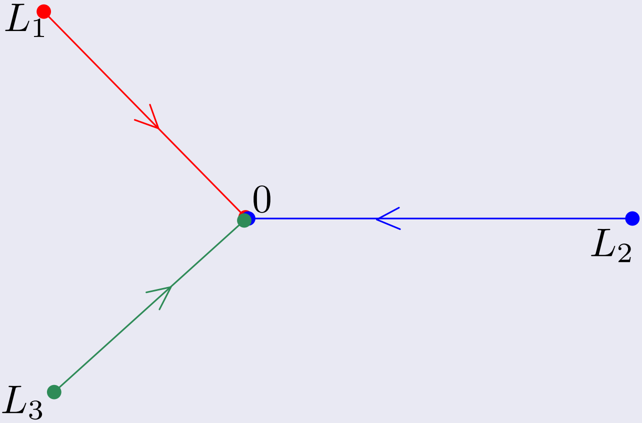


Selfadjointness of $\Delta = \Delta^*$ on $\mathcal{G}$

$$\int_{\mathcal{G}} (-f'')g\,dx = \int_{\mathcal{G}} f(-g'')\,dx$$

Neumann Conditions

Neumann-(Kirchhoff) condition



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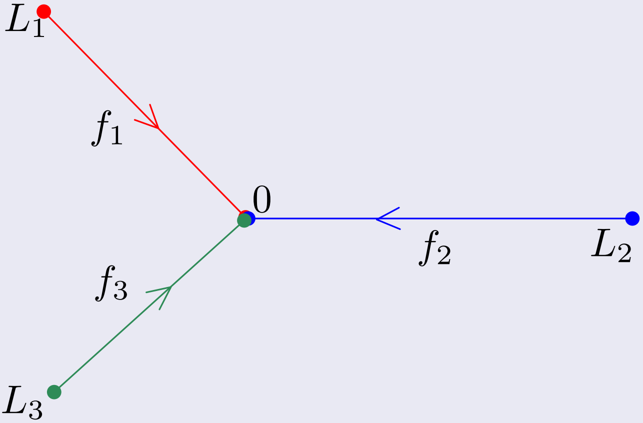

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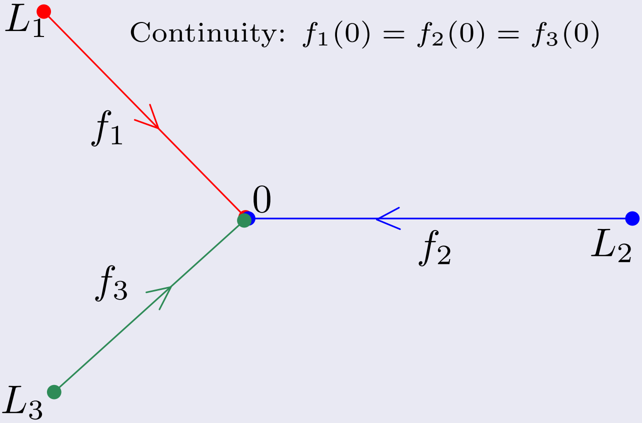

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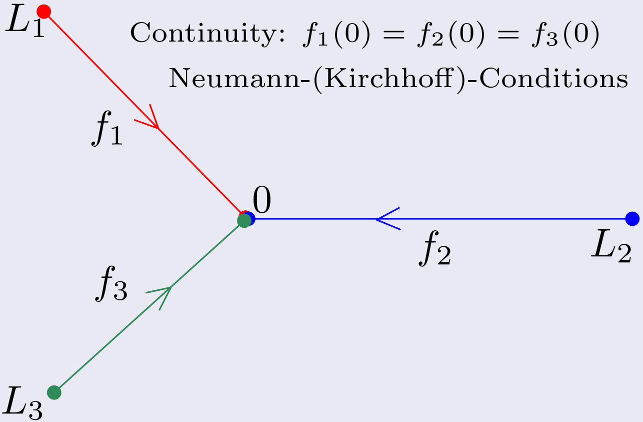

Continuity: $f_1(0) = f_2(0) = f_3(0)$

Neumann-(Kirchhoff)-Conditions

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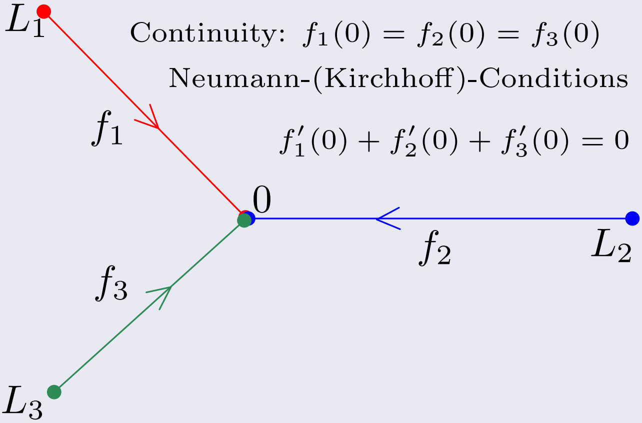

Continuity: $f_1(0) = f_2(0) = f_3(0)$

Neumann-(Kirchhoff)-Conditions

$$f_1'(0) + f_2'(0) + f_3'(0) = 0$$

Neumann vertex condition

Let $f \in L^2(\mathcal{G})$ such that $f_e \in H^2(e)$. We say f satisfies ***Neumann vertex conditions*** if and only if

1. **Continuity:** $f_{e_1}(v) = f_{e_2}(v)$ for all $e_1, e_2 \in \mathcal{E}$ such that $v \in e_1$ and $v \in e_2$.

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2. **Vertex condition:** $\displaystyle\sum_{e: v \in o(e)} f_e'(v) = 0$

Quantum Graph

Theorem - a domain of self-adjointness for Δ

Let $\mathcal{G}$ be a metric graph and $H = \Delta$ be the operator acting as $(\Delta f)_e = -f_e''$ on functions $f_e \in H^2(e)$ with domain

$$\mathrm{Dom}(\Delta) := \left\{ f \in L^2(\mathcal{G}) \mid f_e \in H^2(e) \text{ and } f \text{ satisfies Neumann vertex cond.} \right\}.$$

Then Δ is a self-adjoint operator.

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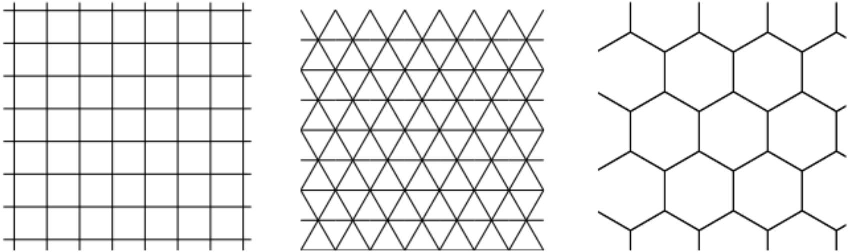
Quantum Graph

The self-adjoint Laplacian Δ on $\mathcal{G}$ is a ***quantum graph***.

$\mathbb{Z}^2$-periodic metric graphs with compact fundamental domain

Embedded planar graphs

For simplicity, we only consider metric graphs that can be thought of as being embeded in $\mathbb{R}^2$ with a fixed geometric structure.

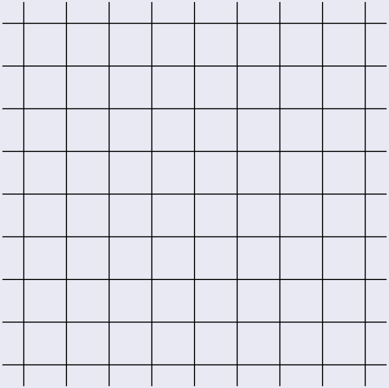


(4^4) (3^6) (6^3)

$\mathbb{Z}^2$-periodic metric graphs with compact fundamental domain

A compact fundamental domain

For every two (linear independent) vectors $w_1, w_2 \in \mathbb{R}^2$ we obtain a finite metric graph, called $\mathcal{Q}$, by only considering what lies inside the parallelogram spanned by w_1 and w_2 at some point $p \in \mathbb{R}^2$.



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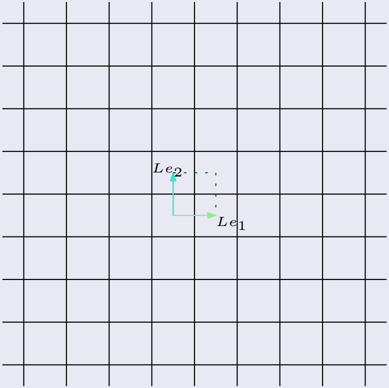

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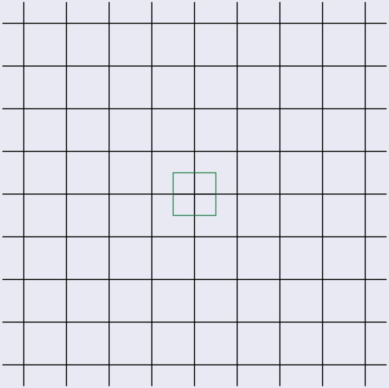

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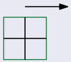
$\mathbb{Z}^2$-periodic metric graphs with compact fundamental domain

$\mathbb{Z}^2$ shifts

A metric graph $\mathcal{G}$ is said to be a $\mathbb{Z}^2$-periodic metric graph if there exists $w_1, w_2 \in \mathbb{R}^2$ such that $\mathcal{G}$ can be recovered by $\mathbb{Z}^2$-shifts along w_1 and w_2.



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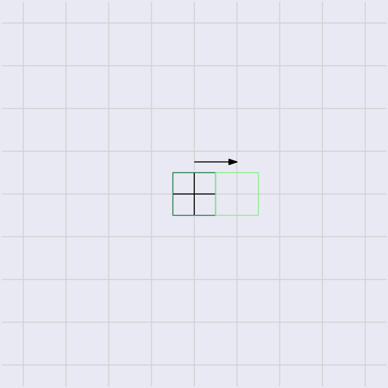

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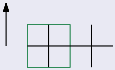

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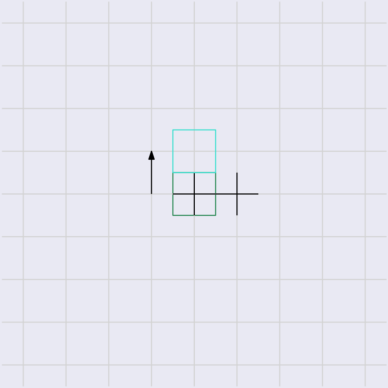

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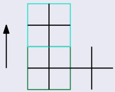

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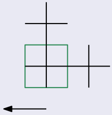

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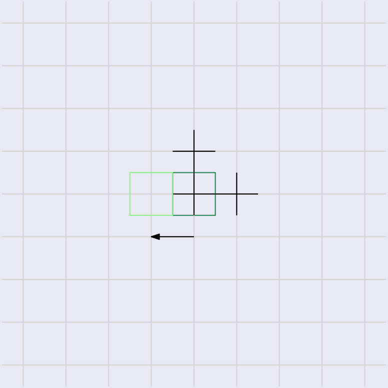

$\mathbb{Z}^2$-periodic metric graphs with compact fundamental domain

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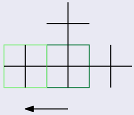

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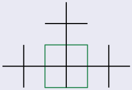

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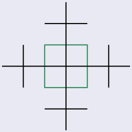

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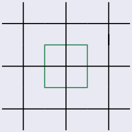

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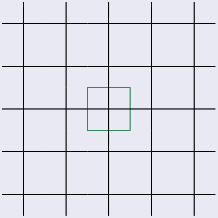

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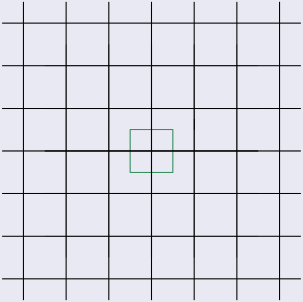

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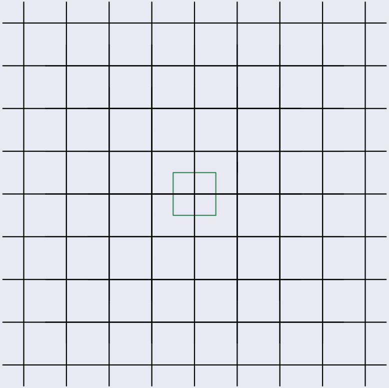
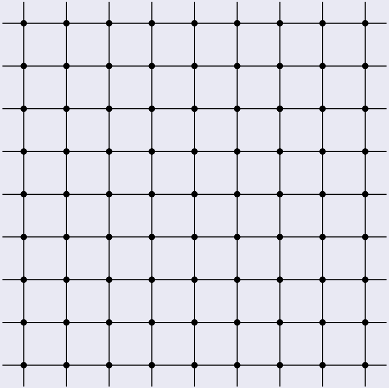


$\mathbb{Z}^2$-periodic metric graphs with compact fundamental domain

The square lattice - our toy example

We consider the infinite square lattice with length L as a quantum graph.



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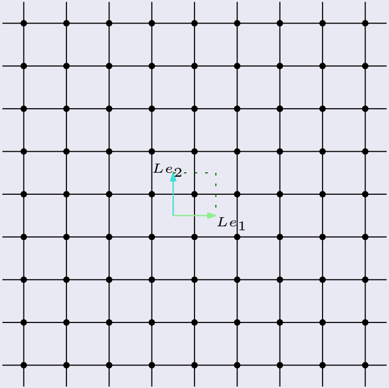
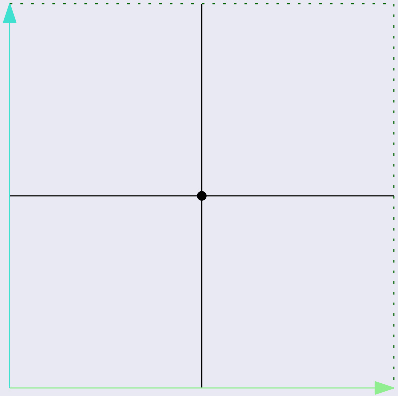


$\mathbb{Z}^2$-periodic metric graphs with compact fundamental domain

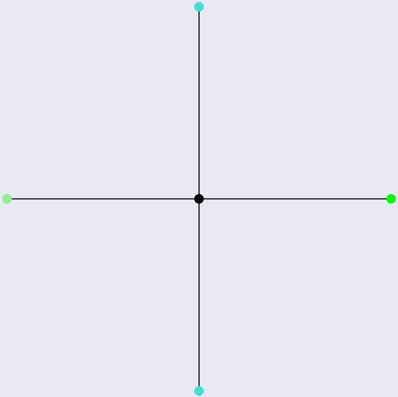
A closer look at the fundamental domain



$\mathbb{Z}^2$-periodic metric graphs with compact fundamental domain

Virtual vertices

We see that the parallelogram cut the edges in half. This introduces 4 new ***virtual*** vertices. Thus, the fundamental domain $\mathcal{Q}$ consists of 5 vertices ...



$\mathbb{Z}^2$-periodic metric graphs with compact fundamental domain

...and 4 edges, each uniquely identified with the interval $[0, L/2]$ with endpoints 0 and $L/2$.

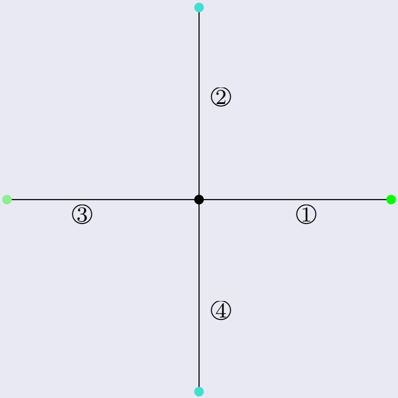


Table of Contents

1 Periodic graphs

2 Floquet Theory

3 Floquet Theory and Periodic Graphs

4 Flat Bands

5 Quantum graphs
- Metric Graphs
- Quantum Graphs
- $\mathbb{Z}^2$-periodic Quantum Graphs

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3. Bringing everything back to the original problem, again by Floquet theory

Floquet Boundary conditions - Quasi Periodicity via the Floquet transform

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$$\mathcal{U} : L^2(\mathcal{Q} \times \mathbb{Z}^2) \to L^2(\mathcal{Q} \times \mathbb{T}^2), \qquad \mathcal{U}f(q,\theta) = \sum_{k \in \mathbb{Z}^2} f(q+k)e^{-ik\theta}.$$

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Note, that for fixed $\theta \in \mathbb{T}^2$ and for (sufficiently regular) $f \in L^2(\mathcal{Q} \times \mathbb{Z}^2)$, the function $\mathcal{Q} \ni q \mapsto (\mathcal{U}f)(q,\theta)$ is θ-quasiperiodic in the sense that

$$(\mathcal{U}f)(q+k,\theta) = (\mathcal{U}f)(q)e^{ik\theta} \qquad \text{for } k \in \mathbb{Z}^2 \text{ such that } q, q+k \in \mathcal{Q},$$

and analougsly for derivatives.

Floquet Neumann vertex condition

Let $\theta \in \mathbb{T}^2$, $f \in L^2(\mathcal{Q})$ such that $f_e \in H^2(e)$. We say f satisfies ***Floquet-Neumann vertex conditions*** at point θ if and only if

1. **(Quasi-)Continuity:** $f_{e_1}(p_{e_1}) = f_{e_2}(p_{e_2})e^{ik_{e_2}\theta}$ for $p_{e_1} = p_{e_2} + k$

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- Let p_0 be an endpoint of some edge in $\mathcal{Q}$. We define

$$\mathcal{E}_{p_0} := \left\{ \begin{array}{l} \text{All the edges } e \text{ with endpoint } p_e \text{ such that there exists} \\ \text{some } k_e \in \mathbb{Z}^2 \text{ so that } p_0 = p_e + k_e \ . \end{array} \right\}$$

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- **Note** that if e_1, e_2 are edges on $\mathcal{Q}$ such that p_0 is both an endpoint of e_1 and e_2, then by the trivial action $\cdot + 0$ we see that $e_1, e_2 \in \mathcal{E}_{p_0}$.

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Proposition

Let $\theta \in \mathbb{T}^2$ and $f \in \mathrm{Dom}(\Delta)$. We write

$$\mathcal{U}_\theta f = \mathcal{U}f(\cdot, \theta).$$

Then $\mathcal{U}_\theta f$ fulfills Floquet-Neumann vertex conditions at point θ.

Floquet Theory - in a Nutshell I

Theorem - Bloch operators Δ_θ

Let $\theta \in \mathbb{T}^2$ and

$$H^2_\theta(\mathcal{Q}) := \left\{ f \in L^2(\mathcal{Q}) \;\middle|\; \begin{array}{l} f_e \in H^2(e) \text{ and } f \text{ satisfies } \textbf{Floquet}\text{-Neumann-} \\ \text{conditions at } \theta \text{ on } \mathcal{Q} \end{array} \right\},$$

and define Δ_θ, as the restriction of Δ to $H^2_\theta(\mathcal{Q})$.

The operator Δ_θ is called the ***Bloch*** *operator*. It is an unbounded self-adjoint operator and its spectrum only consists of (non-negative) eigenvalues.

Floque Theory in a Nutshell

Let Δ be a $\mathbb{Z}^2$-periodic quantum graph on $\mathcal{G}$. Then for $\theta \in \mathbb{T}^2$, we have $\mathcal{U}_\theta f \in \mathrm{Dom}(\Delta_\theta)$ for all $f \in \mathrm{Dom}(\Delta)$, as well as,

$$\Delta(\mathcal{U}f) = \mathcal{U}(\Delta f) \quad \text{and} \quad \mathcal{U}_\theta(\Delta)f = \Delta_\theta(\mathcal{U}_\theta f).$$

Moreover, the spectrum of Δ can be obtained by the spectra of the Bloch operators, i.e

$$\sigma(\Delta) = \bigcup_{\theta\in\mathbb{T}^2} \sigma(\Delta_\theta),$$

and $\lambda \in \sigma(\Delta)$ is an eigenvalue if and only if there exists a non-null set $S \subset \mathbb{T}^2$ such that $\lambda \in \sigma(\Delta_\theta)$ for $\theta \in S$.

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The above states that the Bloch operators are a direct integral decomposition to a unitarily equivalent operator of Δ, i.e.

$$\mathcal{U}\Delta\mathcal{U}^{-1} = \int_{\mathbb{T}^2}^{\oplus} \Delta_\theta d\theta.$$

The Secular Matrix

Let $\mathcal{G}$ be a $\mathbb{Z}^2$-periodic quantum graph with compact fundamental domain $\mathcal{Q}$. Let $n \in \mathbb{N}$ be the number of edges in $\mathcal{Q}$ and denote them by $e_1, \ldots, e_n$.

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Let $\mathcal{G}$ be a $\mathbb{Z}^2$-periodic quantum graph with compact fundamental domain $\mathcal{Q}$. Let $n \in \mathbb{N}$ be the number of edges in $\mathcal{Q}$ and denote them by $e_1, \ldots, e_n$. We are interest in the spectrum of Δ_θ. We therefore solve on each edge the following ODE

$$-u_j'' = E u_j \qquad j = 1, 2, \ldots, n,$$

where $E \in (0, \infty)$, and with general solutions

$$u_j(x) = A_j \cos(\sqrt{E}x) + B_j \sin(\sqrt{E}x).$$

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The case $E = 0$

Note that we excluded 0 in our consideration. In that case we get affine linear functions on each edge. One can see that for non-vanishing constant function, we have $0 \in \sigma(\Delta_\theta)$ for $\theta = 0$.

The Floquet-Neumann boundary conditions provide $2n$ independent conditions to solve for the unknowns $(A_1, \dots, A_n, B_1, \dots, B_n)$. For $\theta \in \mathbb{T}^2$, we have seen that these conditions are of the form

$$u_{e_1}(p_{e_1}) = u_{e_2}(p_{e_2})e^{ik_{e_2}\theta} \quad \text{for } p_{e_1} = p_{e_2} + k$$

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After plugging in the solutions u_j these equations indeed become linear equations in A_j and B_j which still depend on $E \in (0, \infty)$. The corresponding $2n \times 2n$ matrix, denoted by $S_\theta(E)$, is referred to as the ***secular matrix*** of the Δ_θ.

Proposition

The ODE

$$-u_j'' = Eu_j \qquad j = 1, 2, \ldots, n,$$

with the Floquet-Neumann boundary conditions, has a non-trivial solution $u \in \mathrm{Dom}(\Delta_\theta)$ for $E \in (0, \infty)$ *if (and only if)* the secular matrix $S_\theta(E)$ is singular, i.e. if 0 is an eigenvalue.
If $v(\theta)$ is an eigenvector of $S_\theta(E)$ to the eigenvalue 0 with components $v_j(\theta)$, then the corresponding eigenfunction $u \in \mathrm{Dom}(\Delta_\theta)$ is given by

$$u_\nu(x) = v_j(\theta)\cos(\sqrt{E}x) + v_{j+n}(\theta)\sin(\sqrt{E}x) \qquad \text{for } x \in e_\nu.$$

Table of Contents

1. Periodic graphs
2. Floquet Theory
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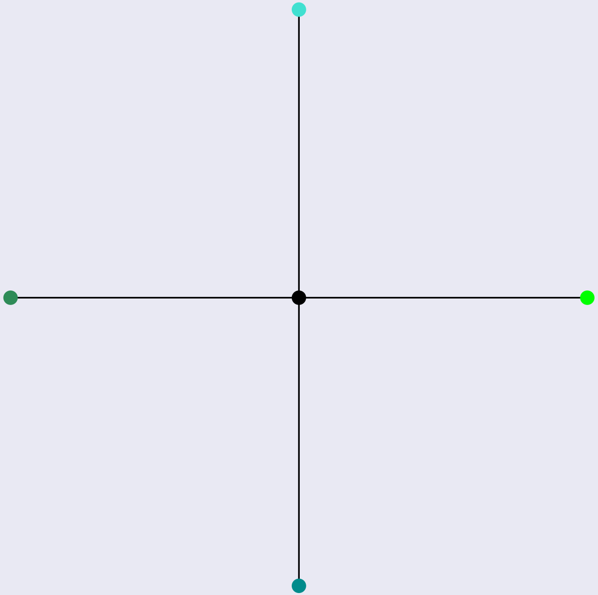

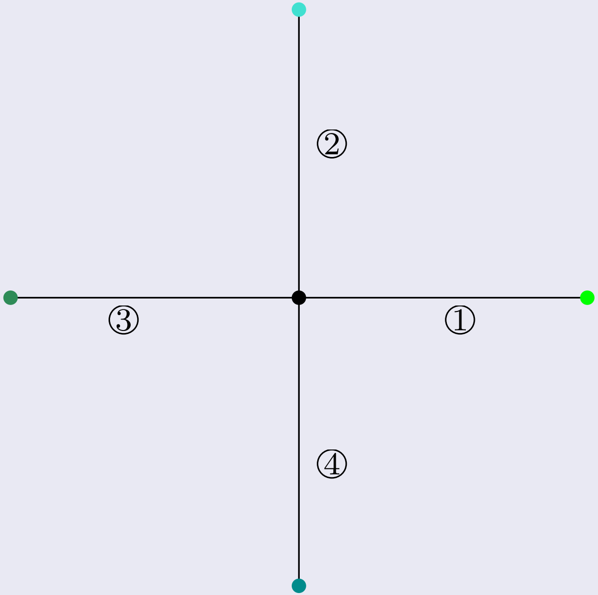
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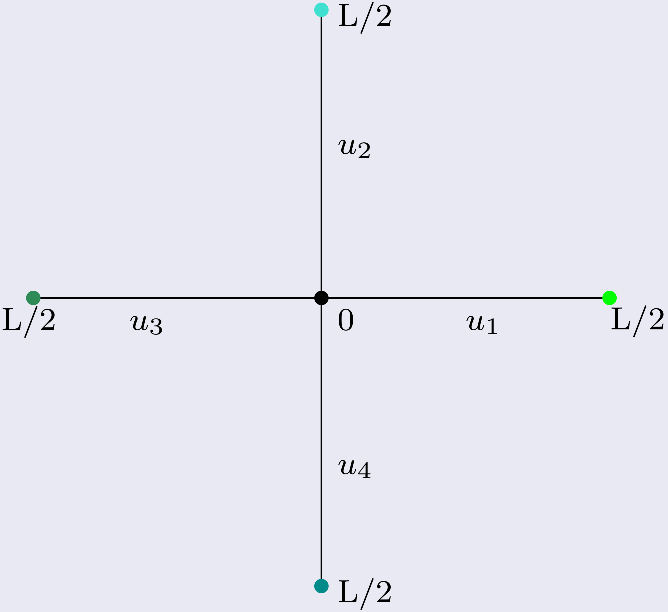
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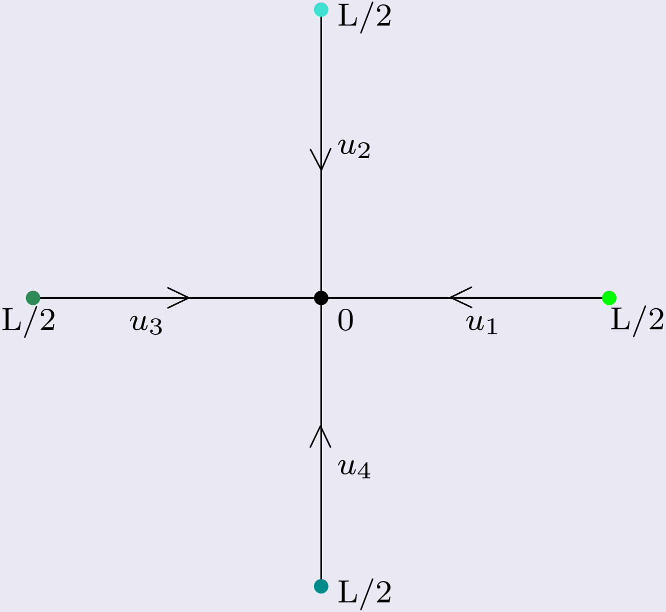
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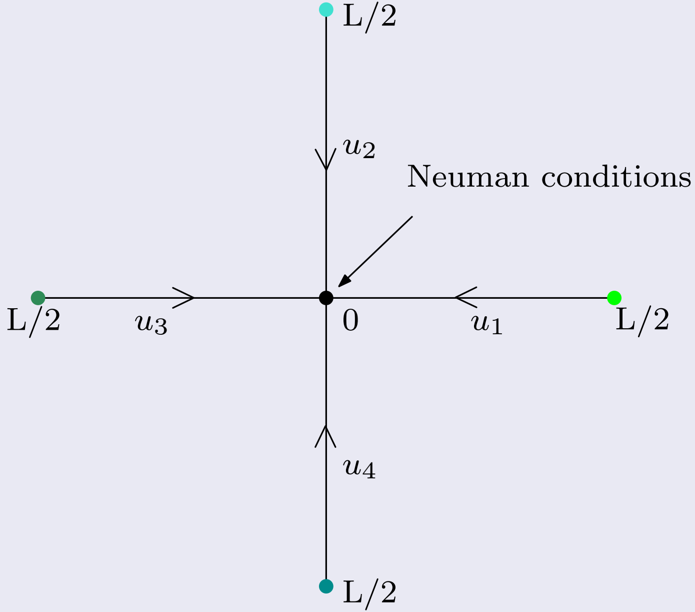
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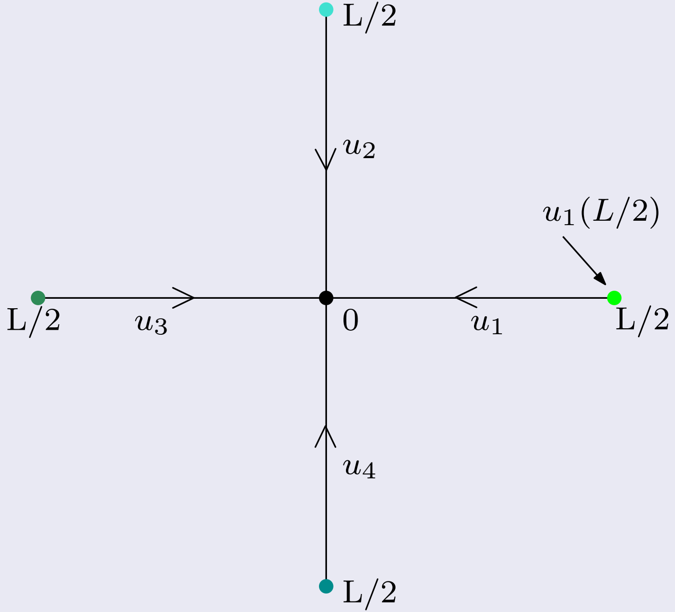
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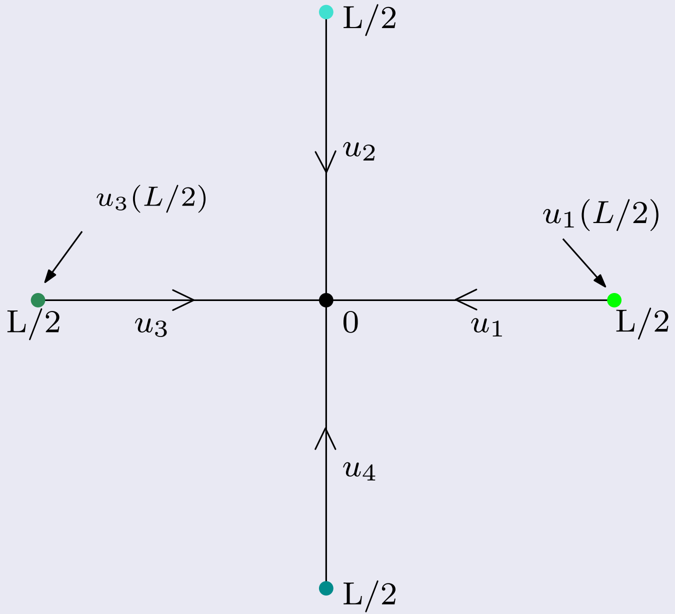
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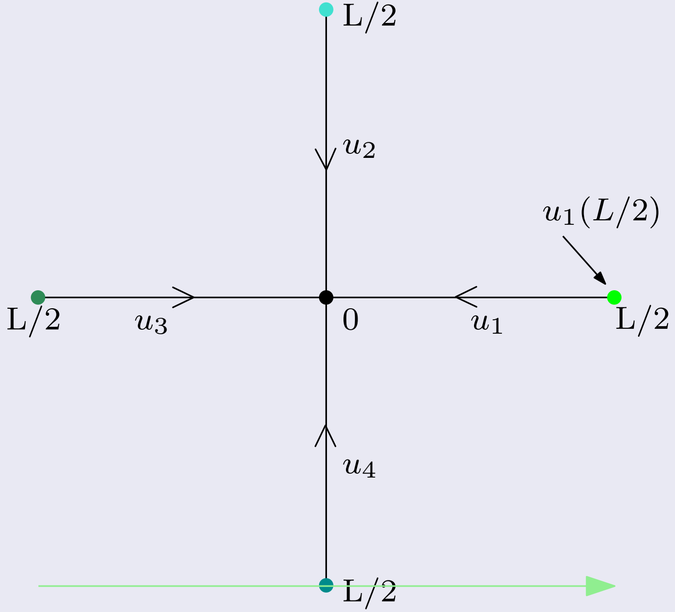
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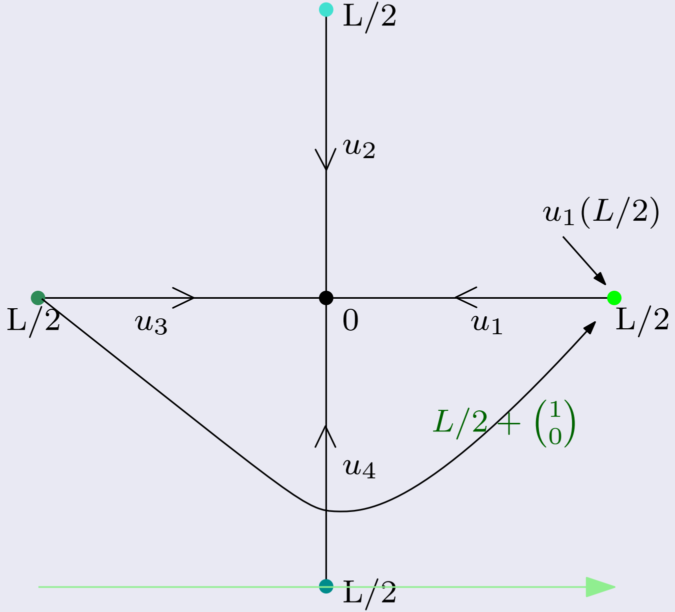
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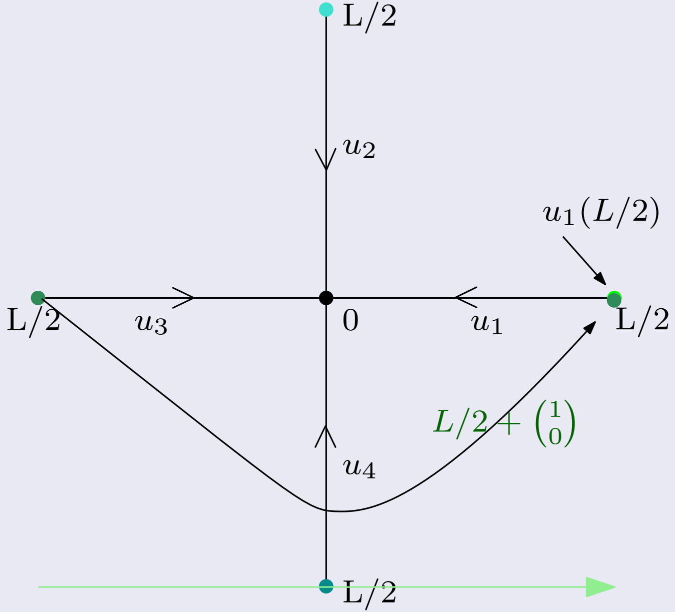
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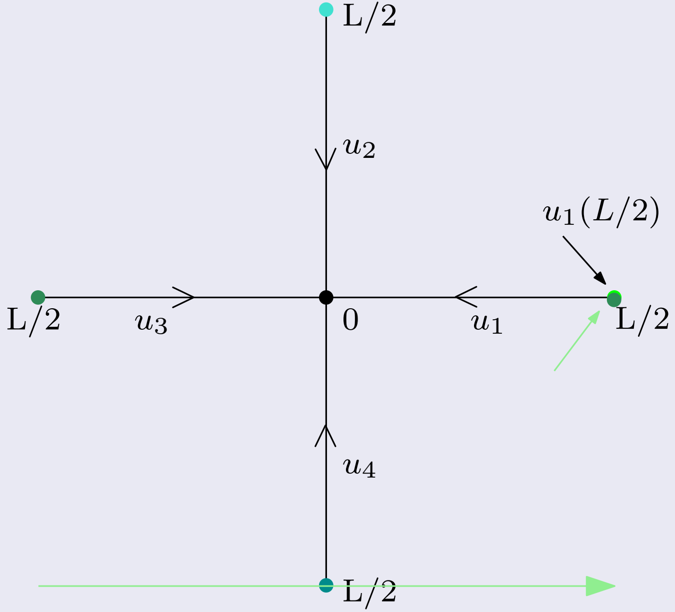
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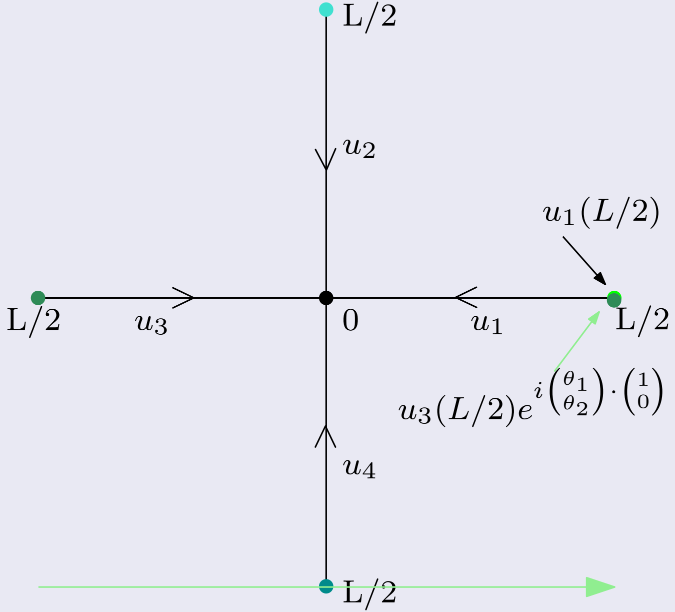
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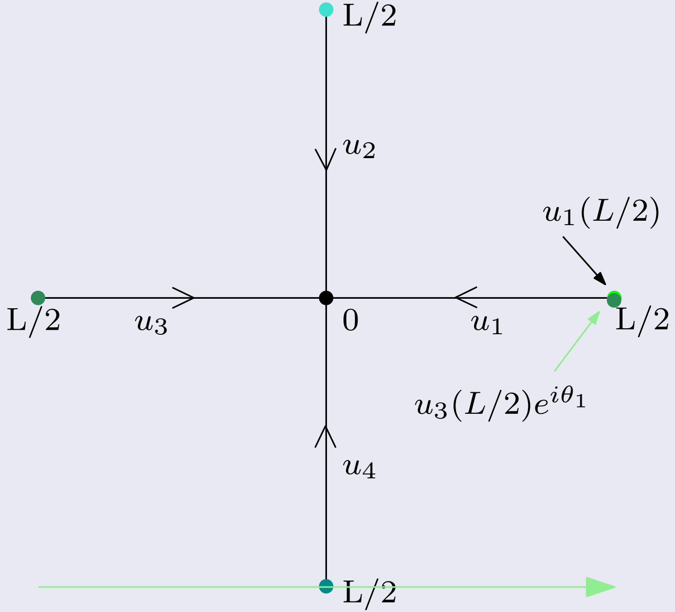
$u_3(L/2)e^{i\begin{pmatrix}\theta_1\\\theta_2\end{pmatrix}\cdot\begin{pmatrix}1\\0\end{pmatrix}}$
u_4
L/2


L/2
u_2
$u_1(L/2)$
L/2
u_3
0
u_1
L/2
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L/2

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These are indeed 8 equation and we can plug in the general solutions

$$u_i(x) = A_i \cos\left(\sqrt{E}x\right) + B_i \sin\left(\sqrt{E}x\right).$$

Solving the secular matrix

We get a linear system in the unknown vector $A_1, \ldots, A_4, B_1 \ldots, B_4$ and the secular matrix becomes

$$\begin{pmatrix} -1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \sqrt{E} & \sqrt{E} & \sqrt{E} & \sqrt{E} \\ -\cos\left(\frac{L\sqrt{E}}{2}\right) & 0 & e^{i\theta_1}\cos\left(\frac{L\sqrt{E}}{2}\right) & 0 & -\sin\left(\frac{L\sqrt{E}}{2}\right) & 0 & e^{i\theta_1}\sin\left(\frac{L\sqrt{E}}{2}\right) & 0 \\ -\sqrt{E}\sin\left(\frac{L\sqrt{E}}{2}\right) & 0 & -\sqrt{E}e^{i\theta_1}\sin\left(\frac{L\sqrt{E}}{2}\right) & 0 & \sqrt{E}\cos\left(\frac{L\sqrt{E}}{2}\right) & 0 & \sqrt{E}e^{i\theta_1}\cos\left(\frac{L\sqrt{E}}{2}\right) & 0 \\ 0 & -\cos\left(\frac{L\sqrt{E}}{2}\right) & 0 & e^{i\theta_2}\cos\left(\frac{L\sqrt{E}}{2}\right) & 0 & -\sin\left(\frac{L\sqrt{E}}{2}\right) & 0 & e^{i\theta_2}\sin\left(\frac{L\sqrt{E}}{2}\right) \\ 0 & -\sqrt{E}\sin\left(\frac{L\sqrt{E}}{2}\right) & 0 & -\sqrt{E}e^{i\theta_2}\sin\left(\frac{L\sqrt{E}}{2}\right) & 0 & \sqrt{E}\cos\left(\frac{L\sqrt{E}}{2}\right) & 0 & \sqrt{E}e^{i\theta_2}\cos\left(\frac{L\sqrt{E}}{2}\right) \end{pmatrix}.$$

We find a non-trivial solution $v \in \mathbb{R}^8$ if and only if the ***the determinant*** of the above matrix vanishes.

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After playing around with python package ***sympy***, we can reduce the determinant for $E \in (0, \infty)$ to

$$\Psi(E;\theta_1,\theta_2) = -2\sqrt{E}^3 2e^{i(\theta_1+\theta_2)}\left(2\cos(L\sqrt{E}) - \cos(\theta_1) - \cos(\theta_2)\right)\sin\left(\frac{L\sqrt{E}}{2}\right)\cos\left(\frac{L\sqrt{E}}{2}\right).$$

Results for the spectra and eigenfunctions

Spectrum of Δ on the square lattice

The spectrum of Δ on the square lattice is

$$\sigma(\Delta) = [0, \infty),$$

where the point spectrum is given by

$$\sigma_p(\Delta) = \{k^2\pi^2 \mid k \in \mathbb{N}\}.$$

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Example of eigenfunctions

For $E = \pi^2$ a corresponding eigenfunction of Δ_θ is of the form

$$u_1(x) = \left(-e^{iv_2} - 1\right) e^{iv_1} \sin\left(\frac{\pi x}{L}\right), \quad u_2(x) = \left(e^{iv_1} + 1\right) e^{iv_2} \sin\left(\frac{\pi x}{L}\right),$$
$$u_3(x) = \left(-e^{iv_2} - 1\right) \sin\left(\frac{\pi x}{L}\right), \quad u_4(x) = \left(e^{iv_1} + 1\right) \sin\left(\frac{\pi x}{L}\right)$$

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Results for metric graph

(An almost proven) Theorem

Consider a $\mathbb{Z}^2$-periodic quantum graph and compact fundamental domain $\mathcal{Q}$. Furthermore, denote by Δ_θ, the Bloch-Hamiltonian, and let $E_0 \in (0, \infty)$. Then the following are equivalent:

1. There exists a measurable set $S \subset \mathbb{T}^2$, $|S| > 0$ such that $E_0 \in \sigma(\Delta_\theta)$ for $\theta \in T$.

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4. There exists infinitely many compactly supported eigenfunction $f \in \mathrm{Dom}(\Delta)$ of Δ for the eigenvalue E_0.

Thank you for your attention !