

Spectra of periodic quantum graphs: more than one would expect

Pavel Exner

Doppler Institute for Mathematical Physics and Applied Mathematics Prague

in collaboration with Daniel Vašata, Miloš Tater, and Ondřej Turek

A talk at the conference Differential Operators on Graphs and Waveguides

Graz, February 25, 2019





It is a standard part of the quantum lore that spectrum of periodic system has a number of familiar properties:

• it is absolutely continuous



- it is absolutely continuous
- it has a *band-and-gap structure*



- it is absolutely continuous
- it has a band-and-gap structure
- in two- or more dimensional systems the *number of open gaps*
 - is always finite by the Bethe-Sommerfled conjecture



- it is absolutely continuous
- it has a band-and-gap structure
- in two- or more dimensional systems the *number of open gaps* is *always finite* by the *Bethe-Sommerfled conjecture*
- *band edges* are reached at the *boundary* of the Brillouin zone or in its *center*



It is a standard part of the quantum lore that spectrum of periodic system has a number of familiar properties:

- it is absolutely continuous
- it has a band-and-gap structure
- in two- or more dimensional systems the *number of open gaps* is *always finite* by the *Bethe-Sommerfled conjecture*
- *band edges* are reached at the *boundary* of the Brillouin zone or in its *center*

My message here is that if the system in question is a quantum graph, *nothing of that needs to be true!*



It is a standard part of the quantum lore that spectrum of periodic system has a number of familiar properties:

- it is absolutely continuous
- it has a band-and-gap structure
- in two- or more dimensional systems the *number of open gaps* is *always finite* by the *Bethe-Sommerfled conjecture*
- *band edges* are reached at the *boundary* of the Brillouin zone or in its *center*

My message here is that if the system in question is a quantum graph, *nothing of that needs to be true!*

To demonstrate this, I am going to discuss *simple examples*, arrays and lattices.



It is a standard part of the quantum lore that spectrum of periodic system has a number of familiar properties:

- it is absolutely continuous
- it has a band-and-gap structure
- in two- or more dimensional systems the *number of open gaps* is *always finite* by the *Bethe-Sommerfled conjecture*
- *band edges* are reached at the *boundary* of the Brillouin zone or in its *center*

My message here is that if the system in question is a quantum graph, *nothing of that needs to be true!*

To demonstrate this, I am going to discuss *simple examples*, arrays and lattices. Should you feel this is not a deep enough mathematics, let me quote a – rather provocative – phrase of Michael Berry:



It is a standard part of the quantum lore that spectrum of periodic system has a number of familiar properties:

- it is absolutely continuous
- it has a band-and-gap structure
- in two- or more dimensional systems the *number of open gaps* is *always finite* by the *Bethe-Sommerfled conjecture*
- *band edges* are reached at the *boundary* of the Brillouin zone or in its *center*

My message here is that if the system in question is a quantum graph, *nothing of that needs to be true!*

To demonstrate this, I am going to discuss *simple examples*, arrays and lattices. Should you feel this is not a deep enough mathematics, let me quote a – rather provocative – phrase of Michael Berry:

Only wimps specialize in the general case. Real scientists pursue examples.



The possible absolute continuity violation comes from the fact that the *unique continuation principle* may not hold in quantum graphs



The possible absolute continuity violation comes from the fact that the *unique continuation principle* may not hold in quantum graphs, where one can encounter the so-called *Dirichlet eigenvalues*



Courtesy: Peter Kuchment

The possible absolute continuity violation comes from the fact that the *unique continuation principle* may not hold in quantum graphs, where one can encounter the so-called *Dirichlet eigenvalues*



Courtesy: Peter Kuchment

The other claims are much less trivial and time will allow just to present results with brief hints about proof ideas

The possible absolute continuity violation comes from the fact that the *unique continuation principle* may not hold in quantum graphs, where one can encounter the so-called *Dirichlet eigenvalues*



Courtesy: Peter Kuchment

The other claims are much less trivial and time will allow just to present results with brief hints about proof ideas

To show that the spectrum may be even *pure point*

The possible absolute continuity violation comes from the fact that the *unique continuation principle* may not hold in quantum graphs, where one can encounter the so-called *Dirichlet eigenvalues*



Courtesy: Peter Kuchment

The other claims are much less trivial and time will allow just to present results with brief hints about proof ideas

To show that the spectrum may be even *pure point* we consider our first example which concerns a *chain graph*

The possible absolute continuity violation comes from the fact that the *unique continuation principle* may not hold in quantum graphs, where one can encounter the so-called *Dirichlet eigenvalues*



Courtesy: Peter Kuchment

The other claims are much less trivial and time will allow just to present results with brief hints about proof ideas

To show that the spectrum may be even *pure point* we consider our first example which concerns a *chain graph* in a *magnetic field*, in general nonconstant

To be specific, the chain graph will look as follows





To be specific, the chain graph will look as follows



The Hamiltonian is *magnetic Laplacian*, $\psi_j \mapsto -\mathcal{D}^2 \psi_j$ on each graph link, where $\mathcal{D} := -i\nabla - \mathbf{A}$



To be specific, the chain graph will look as follows



The Hamiltonian is magnetic Laplacian, $\psi_j \mapsto -\mathcal{D}^2 \psi_j$ on each graph link, where $\mathcal{D} := -i\nabla - \mathbf{A}$, and for definiteness we assume δ -coupling in the vertices, i.e. the domain consists of functions from $H^2_{\text{loc}}(\Gamma)$ satisfying

$$\psi_i(\mathbf{0}) = \psi_j(\mathbf{0}) =: \psi(\mathbf{0}), \quad i, j \in \mathfrak{n}, \quad \sum_{i=1} \mathcal{D}\psi_i(\mathbf{0}) = \alpha \, \psi(\mathbf{0}),$$

п

where $n = \{1, 2, ..., n\}$ is the index set numbering the edges – in our case n = 4 – and $\alpha \in \mathbb{R}$ is the coupling constant



To be specific, the chain graph will look as follows



The Hamiltonian is *magnetic Laplacian*, $\psi_j \mapsto -\mathcal{D}^2 \psi_j$ on each graph link, where $\mathcal{D} := -i\nabla - \mathbf{A}$, and for definiteness we assume δ -coupling in the vertices, i.e. the domain consists of functions from $H^2_{\text{loc}}(\Gamma)$ satisfying

$$\psi_i(\mathbf{0}) = \psi_j(\mathbf{0}) =: \psi(\mathbf{0}), \quad i, j \in \mathfrak{n}, \quad \sum_{i=1} \mathcal{D}\psi_i(\mathbf{0}) = \alpha \, \psi(\mathbf{0}),$$

п

where $n = \{1, 2, ..., n\}$ is the index set numbering the edges – in our case n = 4 – and $\alpha \in \mathbb{R}$ is the coupling constant

This is a particular case of the general conditions that make the operator self-adjoint [Kostrykin-Schrader'03]

DOGW 2019 Graz



We write $\psi_L(x) = e^{-iAx}(C_L^+e^{ikx} + C_L^-e^{-ikx})$ for $x \in [-\pi/2, 0]$ and energy $E := k^2 \neq 0$, and similarly for the other three components



We write $\psi_L(x) = e^{-iAx}(C_L^+e^{ikx} + C_L^-e^{-ikx})$ for $x \in [-\pi/2, 0]$ and energy $E := k^2 \neq 0$, and similarly for the other three components; for *E* negative we put instead $k = i\kappa$ with $\kappa > 0$.



We write $\psi_L(x) = e^{-iAx}(C_L^+e^{ikx} + C_L^-e^{-ikx})$ for $x \in [-\pi/2, 0]$ and energy $E := k^2 \neq 0$, and similarly for the other three components; for *E* negative we put instead $k = i\kappa$ with $\kappa > 0$.

The functions have to be matched through (a) the δ -coupling and



We write $\psi_L(x) = e^{-iAx}(C_L^+e^{ikx} + C_L^-e^{-ikx})$ for $x \in [-\pi/2, 0]$ and energy $E := k^2 \neq 0$, and similarly for the other three components; for *E* negative we put instead $k = i\kappa$ with $\kappa > 0$.

The functions have to be matched through (a) the δ -coupling and (b) Floquet-Bloch conditions. This equation for the phase factor $e^{i\theta}$,

$$\sin k\pi \cos A\pi (e^{2i\theta} - 2\xi(k)e^{i\theta} + 1) = 0$$

with

$$\xi(k) := \frac{1}{\cos A\pi} \Big(\cos k\pi + \frac{\alpha}{4k} \sin k\pi \Big) \,,$$

for any $k \in \mathbb{R} \cup i\mathbb{R} \setminus \{0\}$ and the discriminant equal to $D = 4(\xi(k)^2 - 1)$



We write $\psi_L(x) = e^{-iAx}(C_L^+e^{ikx} + C_L^-e^{-ikx})$ for $x \in [-\pi/2, 0]$ and energy $E := k^2 \neq 0$, and similarly for the other three components; for *E* negative we put instead $k = i\kappa$ with $\kappa > 0$.

The functions have to be matched through (a) the δ -coupling and (b) Floquet-Bloch conditions. This equation for the phase factor $e^{i\theta}$,

$$\sin k\pi \cos A\pi (e^{2i\theta} - 2\xi(k)e^{i\theta} + 1) = 0$$

with

$$\xi(k) := rac{1}{\cos A\pi} \Big(\cos k\pi + rac{lpha}{4k} \sin k\pi \Big) \,,$$

for any $k \in \mathbb{R} \cup i\mathbb{R} \setminus \{0\}$ and the discriminant equal to $D = 4(\xi(k)^2 - 1)$ Apart from the cases $A - \frac{1}{2} \in \mathbb{Z}$ and $k \in \mathbb{N}$ we have $k^2 \in \sigma(-\Delta_{\alpha})$ iff the condition $|\xi(k)| \leq 1$ is satisfied.

P.E.: Spectra of periodic graphs

In picture: determining the spectral bands





The picture refers to A = 0 with $\eta(z) := 4\xi(\sqrt{z})$ and $\gamma = \alpha$

In picture: determining the spectral bands





The picture refers to A = 0 with $\eta(z) := 4\xi(\sqrt{z})$ and $\gamma = \alpha$

For $A - \frac{1}{2} \notin \mathbb{Z}$ the situation is similar, just the width of the band changes to $4 \cos A\pi$, on the other hand, for $A - \frac{1}{2} \in \mathbb{Z}$ it *shrinks to a line*

Duality



The idea was put forward by physicists – *Alexander* and *de Gennes* – and later treated rigorously in [Cattaneo'97], [E'97], and [Pankrashkin'13]

Duality



The idea was put forward by physicists – *Alexander* and *de Gennes* – and later treated rigorously in [Cattaneo'97], [E'97], and [Pankrashkin'13]

We exclude possible Dirichlet eigenvalues from our considerations assuming $k \in \mathfrak{K} := \{z \colon \operatorname{Im} z \ge 0 \land z \notin \mathbb{Z}\}$. On the one hand, we have the differential equation

$$(-\Delta_{\alpha,A}-k^2)\left(egin{array}{c}\psi(x,k)\\\varphi(x,k)\end{array}
ight)=0$$

with the components referring to the upper and lower part of Γ ,

Duality



The idea was put forward by physicists – *Alexander* and *de Gennes* – and later treated rigorously in [Cattaneo'97], [E'97], and [Pankrashkin'13]

We exclude possible Dirichlet eigenvalues from our considerations assuming $k \in \mathfrak{K} := \{z \colon \operatorname{Im} z \ge 0 \land z \notin \mathbb{Z}\}$. On the one hand, we have the differential equation

$$(-\Delta_{\alpha,A}-k^2)\left(egin{array}{c}\psi(x,k)\\\varphi(x,k)\end{array}
ight)=0$$

with the components referring to the upper and lower part of $\Gamma,$ on the other hand the difference one

 $\psi_{j+1}(k)+\psi_{j-1}(k)=\xi_j(k)\psi_j(k)\,,\quad k\in\mathfrak{K}\,,$

where $\psi_j(k) := \psi(j\pi, k)$ and $\xi(k)$ was introduced above, ξ_j corresponding the coupling α_j . The two equations are intimately related.

Duality, continued



Theorem

Let $\alpha_j \in \mathbb{R}$, then any solution $\begin{pmatrix} \psi(\cdot, k) \\ \varphi(\cdot, k) \end{pmatrix}$ with $k^2 \in \mathbb{R}$ and $k \in \mathfrak{K}$ satisfies the difference equation, and conversely, the latter defines via $\begin{pmatrix} \psi(x, k) \\ \varphi(x, k) \end{pmatrix} = e^{\pm iA(x-j\pi)} \Big[\psi_j(k) \cos k(x-j\pi) \Big]$

$$+(\psi_{j+1}(k)\mathrm{e}^{\pm iA\pi}-\psi_j(k)\cos k\pi)\frac{\sin k(x-j\pi)}{\sin k\pi}\Big], \ x\in \left(j\pi,(j+1)\pi\right),$$

solutions to the former satisfying the δ -coupling conditions. In addition, the former belongs to $L^{p}(\Gamma)$ if and only if $\{\psi_{j}(k)\}_{j\in\mathbb{Z}} \in \ell^{p}(\mathbb{Z})$, the claim being true for both $p \in \{2, \infty\}$.

Duality, continued



Theorem

Let $\alpha_j \in \mathbb{R}$, then any solution $\begin{pmatrix} \psi(\cdot, k) \\ \varphi(\cdot, k) \end{pmatrix}$ with $k^2 \in \mathbb{R}$ and $k \in \mathfrak{K}$ satisfies the difference equation, and conversely, the latter defines via $\begin{pmatrix} \psi(x, k) \\ \varphi(x, k) \end{pmatrix} = e^{\mp i A(x-j\pi)} \Big[\psi_j(k) \cos k(x-j\pi) \Big]$

$$+(\psi_{j+1}(k)\mathrm{e}^{\pm i\mathsf{A}\pi}-\psi_j(k)\cos k\pi)\frac{\sin k(x-j\pi)}{\sin k\pi}\bigg], \ x\in \left(j\pi,(j+1)\pi\right),$$

solutions to the former satisfying the δ -coupling conditions. In addition, the former belongs to $L^{p}(\Gamma)$ if and only if $\{\psi_{j}(k)\}_{j\in\mathbb{Z}} \in \ell^{p}(\mathbb{Z})$, the claim being true for both $p \in \{2, \infty\}$.

On can generalize it to other chain graphs, for instance, with varying magnetic field, $A = \{A_j\}_{j \in \mathbb{Z}}$,

Duality, continued



Theorem

Let $\alpha_j \in \mathbb{R}$, then any solution $\begin{pmatrix} \psi(\cdot, k) \\ \varphi(\cdot, k) \end{pmatrix}$ with $k^2 \in \mathbb{R}$ and $k \in \mathfrak{K}$ satisfies the difference equation, and conversely, the latter defines via $\begin{pmatrix} \psi(x, k) \\ \varphi(x, k) \end{pmatrix} = e^{\mp i A(x-j\pi)} \Big[\psi_j(k) \cos k(x-j\pi) \Big]$

$$+(\psi_{j+1}(k)\mathrm{e}^{\pm iA\pi}-\psi_j(k)\cos k\pi)\frac{\sin k(x-j\pi)}{\sin k\pi}\bigg], \ x\in \left(j\pi,(j+1)\pi\right),$$

solutions to the former satisfying the δ -coupling conditions. In addition, the former belongs to $L^{p}(\Gamma)$ if and only if $\{\psi_{j}(k)\}_{j\in\mathbb{Z}} \in \ell^{p}(\mathbb{Z})$, the claim being true for both $p \in \{2, \infty\}$.

On can generalize it to other chain graphs, for instance, with varying magnetic field, $A = \{A_j\}_{j \in \mathbb{Z}}$, the ring (half-)perimeters, $\ell = \{\ell_j\}_{j \in \mathbb{Z}}$, etc.

Example: a single flux altered

It is believed that local perturbations give rise to eigenvalues in the gaps. While often true, it need not be the case generally.

Example: a single flux altered

It is believed that local perturbations give rise to eigenvalues in the gaps. While often true, it need not be the case generally.



We suppose that the field is modified on a single ring, i.e.

 $A = \{\dots, A, A_1, A \dots\}$, the we have a single simple eigenvalue in each gap provided [E-Manko'17]

 $\frac{|\cos A_1\pi|}{|\cos A\pi|}>1\,,$

otherwise the spectrum does not change.

Example: a single flux altered

It is believed that local perturbations give rise to eigenvalues in the gaps. While often true, it need not be the case generally.



We suppose that the field is modified on a single ring, i.e.

 $A = \{\dots, A, A_1, A \dots\}$, the we have a single simple eigenvalue in each gap provided [E-Manko'17]

 $\frac{|\cos A_1\pi|}{|\cos A\pi|} > 1\,,$

otherwise the spectrum does not change.

In particular, the perturbation may give rise to *no eigenvalues in gaps* at all; note that this happens if the perturbed ring is *'further from the non-magnetic case'*
Example: a single flux altered

It is believed that local perturbations give rise to eigenvalues in the gaps. While often true, it need not be the case generally.



We suppose that the field is modified on a single ring, i.e.

 $A = \{\dots, A, A_1, A \dots\}$, the we have a single simple eigenvalue in each gap provided [E-Manko'17]

 $\frac{|\cos A_1\pi|}{|\cos A\pi|} > 1\,,$

otherwise the spectrum does not change.

In particular, the perturbation may give rise to *no eigenvalues in gaps* at all; note that this happens if the perturbed ring is *'further from the non-magnetic case'*

Note also that the eigenvalue may split from the *ac* spectral band of the unperturbed system and lies between this band and the nearest eigenvalue of infinite multiplicity. When we change the magnetic field, the eigenvalue may absorbed in the same band

Example: a single flux altered

It is believed that local perturbations give rise to eigenvalues in the gaps. While often true, it need not be the case generally.



We suppose that the field is modified on a single ring, i.e.

 $A = \{\dots, A, A_1, A \dots\}$, the we have a single simple eigenvalue in each gap provided [E-Manko'17]

 $\frac{|\cos A_1\pi|}{|\cos A\pi|} > 1\,,$

otherwise the spectrum does not change.

In particular, the perturbation may give rise to *no eigenvalues in gaps* at all; note that this happens if the perturbed ring is *'further from the non-magnetic case'*

Note also that the eigenvalue may split from the *ac* spectral band of the unperturbed system and lies between this band and the nearest eigenvalue of infinite multiplicity. When we change the magnetic field, the eigenvalue may absorbed in the same band. On the other hand no eigenvalue emerges from the degenerate band.

P.E.: Spectra of periodic graphs

Can periodic graphs have "wilder" spectra?

Let us first recall the picture everybody knows



Can periodic graphs have "wilder" spectra?

Let us first recall the picture everybody knows





representing the spectrum of the difference operator associated with the *almost Mathieu equation*

$$u_{n+1} + u_{n-1} + 2\lambda \cos(2\pi(\omega + n\alpha))u_n = \epsilon u_n$$

for $\lambda = 1$, otherwise called *Harper equation*, as a function of α

DOGW 2019 Gra



Fractal nature of spectra for electron on a lattice in a homogeneous magnetic field was conjectured by [Azbel'64] but it caught the imagination only after Hofstadter made the structure visible



Fractal nature of spectra for electron on a lattice in a homogeneous magnetic field was conjectured by [Azbel'64] but it caught the imagination only after Hofstadter made the structure visible

It triggered a long and fruitful mathematical quest culminating by the proof of the *Ten Martini Conjecture* by Avila and Jitomirskaya in 2009, that is that the spectrum for an *irrational* field is a *Cantor set*



Fractal nature of spectra for electron on a lattice in a homogeneous magnetic field was conjectured by [Azbel'64] but it caught the imagination only after Hofstadter made the structure visible

It triggered a long and fruitful mathematical quest culminating by the proof of the *Ten Martini Conjecture* by Avila and Jitomirskaya in 2009, that is that the spectrum for an *irrational* field is a *Cantor set*

On the physical side, the effect remained theoretical for a long time and thought of in terms of the mentioned setting, with lattice and and a homogeneous field providing the needed two length scales, generically incommensurable, from the lattice spacing and the cyclotron radius



Fractal nature of spectra for electron on a lattice in a homogeneous magnetic field was conjectured by [Azbel'64] but it caught the imagination only after Hofstadter made the structure visible

It triggered a long and fruitful mathematical quest culminating by the proof of the *Ten Martini Conjecture* by Avila and Jitomirskaya in 2009, that is that the spectrum for an *irrational* field is a *Cantor set*

On the physical side, the effect remained theoretical for a long time and thought of in terms of the mentioned setting, with lattice and and a homogeneous field providing the needed two length scales, generically incommensurable, from the lattice spacing and the cyclotron radius

The first experimental demonstration of such a spectral character was done instead in a microwave waveguide system with suitably placed obstacles simulating the almost Mathieu relation [Kühl et al'98]



Fractal nature of spectra for electron on a lattice in a homogeneous magnetic field was conjectured by [Azbel'64] but it caught the imagination only after Hofstadter made the structure visible

It triggered a long and fruitful mathematical quest culminating by the proof of the *Ten Martini Conjecture* by Avila and Jitomirskaya in 2009, that is that the spectrum for an *irrational* field is a *Cantor set*

On the physical side, the effect remained theoretical for a long time and thought of in terms of the mentioned setting, with lattice and and a homogeneous field providing the needed two length scales, generically incommensurable, from the lattice spacing and the cyclotron radius

The first experimental demonstration of such a spectral character was done instead in a microwave waveguide system with suitably placed obstacles simulating the almost Mathieu relation [Kühl et al'98]

Only recently an experimental realization of the original concept was achieved using a graphene lattice [Dean et al'13], [Ponomarenko'13]

Suppose that $A_j = \alpha j + \theta$ holds for some $\alpha, \theta \in \mathbb{R}$ and every $j \in \mathbb{Z}$



Suppose that $A_j = \alpha j + \theta$ holds for some $\alpha, \theta \in \mathbb{R}$ and every $j \in \mathbb{Z}$



We need a stronger version of duality proved in [Pankrashkin'13] using boundary triples: we exclude $\sigma_D = \{k^2 : k \in \mathbb{N}\}$ and introduce

 $s(x;z) = \begin{cases} \frac{\sin(x\sqrt{z})}{\sqrt{z}} & \text{for } z \neq 0, \\ x & \text{for } z = 0, \end{cases} \quad \text{and} \quad c(x;z) = \cos(x\sqrt{z})$

Suppose that $A_j = \alpha j + \theta$ holds for some $\alpha, \theta \in \mathbb{R}$ and every $j \in \mathbb{Z}$



We need a stronger version of duality proved in [Pankrashkin'13] using boundary triples: we exclude $\sigma_D = \{k^2 : k \in \mathbb{N}\}$ and introduce

 $s(x;z) = \begin{cases} \frac{\sin(x\sqrt{z})}{\sqrt{z}} & \text{for } z \neq 0, \\ x & \text{for } z = 0, \end{cases} \quad \text{and} \quad c(x;z) = \cos(x\sqrt{z})$

Theorem (after Pankrashkin'13)

For any interval $J \subset \mathbb{R} \setminus \sigma_D$, the operator $(H_{\gamma,A})_J$ is unitarily equivalent to the pre-image $\eta^{(-1)}((L_A)_{\eta(J)})$, where L_A is the operator on $\ell^2(\mathbb{Z})$ acting as $(L_A q \varphi)_j = 2 \cos(A_j \pi) \varphi_{j+1} + 2 \cos(A_{j-1} \pi) \varphi_{j-1}$ and

 $\eta(z) := \gamma s(\pi; z) + 2c(\pi; z) + 2s'(\pi; z)$

Suppose that $A_j = \alpha j + \theta$ holds for some $\alpha, \theta \in \mathbb{R}$ and every $j \in \mathbb{Z}$



We need a stronger version of duality proved in [Pankrashkin'13] using boundary triples: we exclude $\sigma_D = \{k^2 : k \in \mathbb{N}\}$ and introduce

 $s(x;z) = \begin{cases} \frac{\sin(x\sqrt{z})}{\sqrt{z}} & \text{for } z \neq 0, \\ x & \text{for } z = 0, \end{cases} \quad \text{and} \quad c(x;z) = \cos(x\sqrt{z})$

Theorem (after Pankrashkin'13)

For any interval $J \subset \mathbb{R} \setminus \sigma_D$, the operator $(H_{\gamma,A})_J$ is unitarily equivalent to the pre-image $\eta^{(-1)}((L_A)_{\eta(J)})$, where L_A is the operator on $\ell^2(\mathbb{Z})$ acting as $(L_A q \varphi)_j = 2 \cos(A_j \pi) \varphi_{j+1} + 2 \cos(A_{j-1} \pi) \varphi_{j-1}$ and $\eta(z) := \gamma s(\pi; z) + 2c(\pi; z) + 2s'(\pi; z)$

Important: a simple gauge transformation shows that it is only the *fractional part of* A_i which matters

Suppose that $A_j = \alpha j + \theta$ holds for some $\alpha, \theta \in \mathbb{R}$ and every $j \in \mathbb{Z}$



We need a stronger version of duality proved in [Pankrashkin'13] using boundary triples: we exclude $\sigma_D = \{k^2 : k \in \mathbb{N}\}$ and introduce

 $s(x;z) = \begin{cases} \frac{\sin(x\sqrt{z})}{\sqrt{z}} & \text{for } z \neq 0, \\ x & \text{for } z = 0, \end{cases} \quad \text{and} \quad c(x;z) = \cos(x\sqrt{z})$

Theorem (after Pankrashkin'13)

For any interval $J \subset \mathbb{R} \setminus \sigma_D$, the operator $(H_{\gamma,A})_J$ is unitarily equivalent to the pre-image $\eta^{(-1)}((L_A)_{\eta(J)})$, where L_A is the operator on $\ell^2(\mathbb{Z})$ acting as $(L_A q \varphi)_j = 2 \cos(A_j \pi) \varphi_{j+1} + 2 \cos(A_{j-1} \pi) \varphi_{j-1}$ and

 $\eta(z) := \gamma s(\pi; z) + 2c(\pi; z) + 2s'(\pi; z)$

Important: a simple gauge transformation shows that it is only the *fractional part of A_j* which matters. Consequently, the case of a *rational slope*, $\alpha = p/q$, is reduced to a periodic problem allowing the usual Floquet-Bloch treatment

P.E.: Spectra of periodic graphs



For *irrational slope* duality allows to transform the problem into Harpe equation. In this way we get *in a cheap way* a rather nontrivial result:



For *irrational slope* duality allows to transform the problem into Harpek equation. In this way we get *in a cheap way* a rather nontrivial result:

Theorem (E-Vašata'17)

Let $A_j = \alpha j + \theta$ for some $\alpha, \theta \in \mathbb{R}$ and every $j \in \mathbb{Z}$. Then for the spectrum $\sigma(-\Delta_{\gamma,A})$ the following holds:

arpe

For *irrational slope* duality allows to transform the problem into Harpek equation. In this way we get *in a cheap way* a rather nontrivial result:

Theorem (E-Vašata'17)

Let $A_j = \alpha j + \theta$ for some $\alpha, \theta \in \mathbb{R}$ and every $j \in \mathbb{Z}$. Then for the spectrum $\sigma(-\Delta_{\gamma,A})$ the following holds:

(a) If $\alpha, \theta \in \mathbb{Z}$ and $\gamma = 0$, then $\sigma_{ac}(-\Delta_{\gamma,A}) = [0,\infty)$ and $\sigma_{pp}(-\Delta_{\gamma,A}) = \{n^2 | n \in \mathbb{N}\}$

arpe

For *irrational slope* duality allows to transform the problem into Harpel equation. In this way we get *in a cheap way* a rather nontrivial result:

Theorem (E-Vašata'17)

Let $A_j = \alpha j + \theta$ for some $\alpha, \theta \in \mathbb{R}$ and every $j \in \mathbb{Z}$. Then for the spectrum $\sigma(-\Delta_{\gamma,A})$ the following holds:

(a) If $\alpha, \theta \in \mathbb{Z}$ and $\gamma = 0$, then $\sigma_{ac}(-\Delta_{\gamma,A}) = [0,\infty)$ and $\sigma_{pp}(-\Delta_{\gamma,A}) = \{n^2 | n \in \mathbb{N}\}$

(b) If $\gamma \neq 0$ and $\alpha = p/q$ with p, q relatively prime, $\alpha j + \theta + \frac{1}{2} \notin \mathbb{Z}$ for all j = 0, ..., q - 1, then $-\Delta_{\gamma,A}$ has infinitely degenerate ev's $\{n^2 | n \in \mathbb{N}\}$ interlaced with an ac part consisting of q-tuples of closed intervals

arpe

For *irrational slope* duality allows to transform the problem into Harpek equation. In this way we get *in a cheap way* a rather nontrivial result:

Theorem (E-Vašata'17)

Let $A_j = \alpha j + \theta$ for some $\alpha, \theta \in \mathbb{R}$ and every $j \in \mathbb{Z}$. Then for the spectrum $\sigma(-\Delta_{\gamma,A})$ the following holds:

(a) If $\alpha, \theta \in \mathbb{Z}$ and $\gamma = 0$, then $\sigma_{ac}(-\Delta_{\gamma,A}) = [0,\infty)$ and $\sigma_{pp}(-\Delta_{\gamma,A}) = \{n^2 | n \in \mathbb{N}\}$

(b) If $\gamma \neq 0$ and $\alpha = p/q$ with p, q relatively prime, $\alpha j + \theta + \frac{1}{2} \notin \mathbb{Z}$ for all j = 0, ..., q - 1, then $-\Delta_{\gamma,A}$ has infinitely degenerate ev's $\{n^2 | n \in \mathbb{N}\}$ interlaced with an ac part consisting of q-tuples of closed intervals

(c) If the situation is as in (b) but $\alpha j + \theta + \frac{1}{2} \in \mathbb{Z}$ holds for some $j = 0, \ldots, q - 1$, then the spectrum $\sigma(-\Delta_{\gamma,A})$ consists of infinitely degenerate eigenvalues only, the Dirichlet ones plus q distinct others in each interval $(-\infty, 1)$ and $(n^2, (n + 1)^2)$.

The chain graph spectrum, continued



Theorem (E-Vašata'17, cont'd)

(d) If $\gamma \neq 0$ and $\alpha \notin \mathbb{Q}$, then $\sigma(-\Delta_{\gamma,A})$ does not depend on θ and it is a disjoint union of the isolated-point family $\{n^2 | n \in \mathbb{N}\}$ and Cantor sets, one inside each interval $(-\infty, 1)$ and $(n^2, (n+1)^2)$, $n \in \mathbb{N}$. Moreover, the overall Lebesgue measure of $\sigma(-\Delta_{\gamma,A})$ is zero.

The chain graph spectrum, continued



Theorem (E-Vašata'17, cont'd)

(d) If $\gamma \neq 0$ and $\alpha \notin \mathbb{Q}$, then $\sigma(-\Delta_{\gamma,A})$ does not depend on θ and it is a disjoint union of the isolated-point family $\{n^2 | n \in \mathbb{N}\}$ and Cantor sets, one inside each interval $(-\infty, 1)$ and $(n^2, (n+1)^2)$, $n \in \mathbb{N}$. Moreover, the overall Lebesgue measure of $\sigma(-\Delta_{\gamma,A})$ is zero.

Furthermore, using a result of [Last-Shamis'16] one can also show

Proposition

Let $A_j = \alpha j + \theta$ for some $\alpha, \theta \in \mathbb{R}$ and every $j \in \mathbb{Z}$. There exist a dense G_{δ} set of the slopes α for which, and all θ , the Haussdorff dimension

 $\dim_H \sigma(-\Delta_{\gamma,A}) = 0$



The graphs in the previous example had 'many' gaps indeed. Let us now ask whether periodic graphs can have 'just a few' gaps



The graphs in the previous example had 'many' gaps indeed. Let us now ask whether periodic graphs can have 'just a few' gaps

For 'ordinary' Schrödinger operators the dimension is decisive



The graphs in the previous example had 'many' gaps indeed. Let us now ask whether periodic graphs can have 'just a few' gaps

For 'ordinary' Schrödinger operators the dimension is decisive: the systems which are \mathbb{Z} -periodic have generically an infinite number of open gaps,



The graphs in the previous example had 'many' gaps indeed. Let us now ask whether periodic graphs can have 'just a few' gaps

For 'ordinary' Schrödinger operators the dimension is decisive: the systems which are \mathbb{Z} -periodic have generically an infinite number of open gaps, while \mathbb{Z}^{ν} -periodic systems with $\nu \geq 2$ have only finitely many open gaps



The graphs in the previous example had 'many' gaps indeed. Let us now ask whether periodic graphs can have 'just a few' gaps

For 'ordinary' Schrödinger operators the dimension is decisive: the systems which are \mathbb{Z} -periodic have generically an infinite number of open gaps, while \mathbb{Z}^{ν} -periodic systems with $\nu \geq 2$ have only finitely many open gaps

This is the celebrated *Bethe–Sommerfeld conjecture* to which we have nowadays an affirmative answer in a large number of cases



The graphs in the previous example had 'many' gaps indeed. Let us now ask whether periodic graphs can have 'just a few' gaps

For 'ordinary' Schrödinger operators the dimension is decisive: the systems which are \mathbb{Z} -periodic have generically an infinite number of open gaps, while \mathbb{Z}^{ν} -periodic systems with $\nu \geq 2$ have only finitely many open gaps

This is the celebrated *Bethe–Sommerfeld conjecture* to which we have nowadays an affirmative answer in a large number of cases

In quantum graphs, *'this is not a strict law'* by [Berkolaiko-Kuchment'13]. For instance, we know that infinitely many gaps can by created by a *graph 'decoration'*, cf. [Schenker-Aizenman'00], [Kuchment'04]



The graphs in the previous example had 'many' gaps indeed. Let us now ask whether periodic graphs can have 'just a few' gaps

For 'ordinary' Schrödinger operators the dimension is decisive: the systems which are \mathbb{Z} -periodic have generically an infinite number of open gaps, while \mathbb{Z}^{ν} -periodic systems with $\nu \geq 2$ have only finitely many open gaps

This is the celebrated *Bethe–Sommerfeld conjecture* to which we have nowadays an affirmative answer in a large number of cases

In quantum graphs, *'this is not a strict law'* by [Berkolaiko-Kuchment'13]. For instance, we know that infinitely many gaps can by created by a *graph 'decoration'*, cf. [Schenker-Aizenman'00], [Kuchment'04]

The question arises, whether it is a 'law' at all?. In other words, do infinite periodic graphs having a *finite nonzero* number of open gaps exist?



The graphs in the previous example had 'many' gaps indeed. Let us now ask whether periodic graphs can have 'just a few' gaps

For 'ordinary' Schrödinger operators the dimension is decisive: the systems which are \mathbb{Z} -periodic have generically an infinite number of open gaps, while \mathbb{Z}^{ν} -periodic systems with $\nu \geq 2$ have only finitely many open gaps

This is the celebrated *Bethe–Sommerfeld conjecture* to which we have nowadays an affirmative answer in a large number of cases

In quantum graphs, *'this is not a strict law'* by [Berkolaiko-Kuchment'13]. For instance, we know that infinitely many gaps can by created by a *graph 'decoration'*, cf. [Schenker-Aizenman'00], [Kuchment'04]

The question arises, whether it is a 'law' at all?. In other words, do infinite periodic graphs having a *finite nonzero* number of open gaps exist? From obvious reasons we would call them *Bethe–Sommerfeld graphs*

Scale-invariant coupling



The answer depends on the vertex coupling. Recall that the standard conditions for self-adjoint coupling of n edges at a vertex,

 $(U-I)\Psi+i(U+I)\Psi'=0,$

where U is an $n \times n$ unitary matrix

Scale-invariant coupling



The answer depends on the vertex coupling. Recall that the standard conditions for self-adjoint coupling of n edges at a vertex,

 $(U-I)\Psi+i(U+I)\Psi'=0\,,$

where U is an $n \times n$ unitary matrix. They decomposes into Dirichlet, Neumann, and Robin parts corresponding to eigenspaces of U with eigenvalues -1, 1, and the rest, respectively; if the latter is absent we call such a coupling *scale-invariant*

Scale-invariant coupling



The answer depends on the vertex coupling. Recall that the standard conditions for self-adjoint coupling of n edges at a vertex,

 $(U-I)\Psi+i(U+I)\Psi'=0\,,$

where U is an $n \times n$ unitary matrix. They decomposes into Dirichlet, Neumann, and Robin parts corresponding to eigenspaces of U with eigenvalues -1, 1, and the rest, respectively; if the latter is absent we call such a coupling *scale-invariant*

Theorem ([E-Turek'17])

An infinite periodic quantum graph does not belong to the Bethe-Sommerfeld class if the couplings at its vertices are scale-invariant.



The spectrum is determined by *secular equation* [BB'15]: we define

$$\mathsf{F}(k;ec{ec{ec{v}}}):=\det\left(\mathsf{I}-\mathrm{e}^{i(\mathbf{A}+k\mathbf{L})}\mathbf{S}(k)
ight),$$

where the $2E \times 2E$ matrices **A**, **L**, and **S** are as follows: the diagonal matrix **L** is given by the lengths of the directed edges (bonds) of Γ ,



The spectrum is determined by *secular equation* [BB'15]: we define

$$\mathcal{F}(k; ec{ec{ec{v}}}) := \det \left(\mathsf{I} - \mathrm{e}^{i(\mathbf{A}+k\mathsf{L})} \mathsf{S}(k)
ight),$$

where the $2E \times 2E$ matrices **A**, **L**, and **S** are as follows: the diagonal matrix **L** is given by the lengths of the directed edges (bonds) of Γ , the diagonal **A** has entries $e^{\pm i\vartheta_I}$ at points of the 'Brillouin torus identification', all the others are zero



The spectrum is determined by *secular equation* [BB'15]: we define

$$\mathcal{F}(k; ec{ec{ec{v}}}) := \det \left(\mathsf{I} - \mathrm{e}^{i(\mathbf{A}+k\mathsf{L})} \mathsf{S}(k)
ight),$$

where the $2E \times 2E$ matrices **A**, **L**, and **S** are as follows: the diagonal matrix **L** is given by the lengths of the directed edges (bonds) of Γ , the diagonal **A** has entries $e^{\pm i\vartheta_I}$ at points of the 'Brillouin torus identification', all the others are zero, and finally, **S** is the *bond scattering matrix*



The spectrum is determined by *secular equation* [BB'15]: we define

$$\mathcal{F}(k;ec{ec{ec{v}}}):=\det\left(\mathsf{I}-\mathrm{e}^{i(\mathbf{A}+k\mathsf{L})}\mathsf{S}(k)
ight) ,$$

where the $2E \times 2E$ matrices **A**, **L**, and **S** are as follows: the diagonal matrix **L** is given by the lengths of the directed edges (bonds) of Γ , the diagonal **A** has entries $e^{\pm i\vartheta_I}$ at points of the 'Brillouin torus identification', all the others are zero, and finally, **S** is the *bond scattering matrix*

Then $k^2 \in \sigma(H)$ holds if there is a quasimomentum values $\vec{\vartheta} \in (-\pi, \pi]^{\nu}$) such that the equation $F(k; \vec{\vartheta}) = 0$ is satisfied
Proof idea



The spectrum is determined by *secular equation* [BB'15]: we define

$$\mathcal{F}(k; ec{ec{ec{v}}}) := \det \left(\mathbf{I} - \mathrm{e}^{i(\mathbf{A}+k\mathbf{L})} \mathbf{S}(k)
ight),$$

where the $2E \times 2E$ matrices **A**, **L**, and **S** are as follows: the diagonal matrix **L** is given by the lengths of the directed edges (bonds) of Γ , the diagonal **A** has entries $e^{\pm i \vartheta_I}$ at points of the 'Brillouin torus identification', all the others are zero, and finally, **S** is the *bond scattering matrix*

Then $k^2 \in \sigma(H)$ holds if there is a quasimomentum values $\vec{\vartheta} \in (-\pi, \pi]^{\nu}$) such that the equation $F(k; \vec{\vartheta}) = 0$ is satisfied

We note that $F(k; \vec{\vartheta} \text{ depends on } \vec{\vartheta} \text{ and } (k\ell_0, k\ell_1, \dots, k\ell_d)$, where $\{\ell_0, \ell_1, \dots, \ell_d\}, d+1 \leq E$ are the mutually different edge lengths of Γ

Proof idea



The spectrum is determined by *secular equation* [BB'15]: we define

$$\mathcal{F}(k; ec{ec{ec{v}}}) := \det \left(\mathbf{I} - \mathrm{e}^{i(\mathbf{A}+k\mathbf{L})} \mathbf{S}(k)
ight),$$

where the $2E \times 2E$ matrices **A**, **L**, and **S** are as follows: the diagonal matrix **L** is given by the lengths of the directed edges (bonds) of Γ , the diagonal **A** has entries $e^{\pm i \vartheta_I}$ at points of the 'Brillouin torus identification', all the others are zero, and finally, **S** is the *bond scattering matrix*

Then $k^2 \in \sigma(H)$ holds if there is a quasimomentum values $\vec{\vartheta} \in (-\pi, \pi]^{\nu}$) such that the equation $F(k; \vec{\vartheta}) = 0$ is satisfied

We note that $F(k; \vec{\vartheta} \text{ depends on } \vec{\vartheta} \text{ and } (k\ell_0, k\ell_1, \dots, k\ell_d)$, where $\{\ell_0, \ell_1, \dots, \ell_d\}, d+1 \leq E$ are the mutually different edge lengths of Γ . If the ℓ 's are rationally related, the function is *periodic* in k, hence if there is a gap, there are *infinitely many of them*

If the lengths are *not* rationally related, their ratios can be *approximated by rationals* with an arbitrary precision.

If the lengths are *not* rationally related, their ratios can be *approximated by rationals* with an arbitrary precision.

If k^2 is in a gap, i.e. $|F(k; \vec{\vartheta})| > \delta$ for some $\delta > 0$ and all $\vec{\vartheta} \in (-\pi, \pi]^{\nu}$)

If the lengths are *not* rationally related, their ratios can be *approximated* by *rationals* with an arbitrary precision.

If k^2 is in a gap, i.e. $|F(k; \vec{\vartheta})| > \delta$ for some $\delta > 0$ and all $\vec{\vartheta} \in (-\pi, \pi]^{\nu}$) – recall that $|F(k; \cdot))|$ has a minimum at the torus –

If the lengths are *not* rationally related, their ratios can be *approximated by rationals* with an arbitrary precision.

If k^2 is in a gap, i.e. $|F(k; \vec{\vartheta})| > \delta$ for some $\delta > 0$ and all $\vec{\vartheta} \in (-\pi, \pi]^{\nu})$ – recall that $|F(k; \cdot))|$ has a minimum at the torus – then its value will remain separated from zero when the ℓ 's are replaced by the rational approximants and k is large enough. \Box

If the lengths are *not* rationally related, their ratios can be *approximated by rationals* with an arbitrary precision.

If k^2 is in a gap, i.e. $|F(k; \vec{\vartheta})| > \delta$ for some $\delta > 0$ and all $\vec{\vartheta} \in (-\pi, \pi]^{\nu})$ – recall that $|F(k; \cdot))|$ has a minimum at the torus – then its value will remain separated from zero when the ℓ 's are replaced by the rational approximants and k is large enough. \Box

Recall next that the vertex conditions can be equivalently written as

$$\left(\begin{array}{cc}I^{(r)}&T\\0&0\end{array}\right)\Psi'=\left(\begin{array}{cc}S&0\\-T^*&I^{(n-r)}\end{array}\right)\Psi$$

for certain r, S, and T, where $I^{(r)}$ is the identity matrix of order r; the coupling is scale-invariant if and only if the square matrix S = 0

If the lengths are *not* rationally related, their ratios can be *approximated* by *rationals* with an arbitrary precision.

If k^2 is in a gap, i.e. $|F(k; \vec{\vartheta})| > \delta$ for some $\delta > 0$ and all $\vec{\vartheta} \in (-\pi, \pi]^{\nu})$ – recall that $|F(k; \cdot))|$ has a minimum at the torus – then its value will remain separated from zero when the ℓ 's are replaced by the rational approximants and k is large enough. \Box

Recall next that the vertex conditions can be equivalently written as

$$\left(\begin{array}{cc}I^{(r)}&T\\0&0\end{array}\right)\Psi'=\left(\begin{array}{cc}S&0\\-T^*&I^{(n-r)}\end{array}\right)\Psi$$

for certain r, S, and T, where $I^{(r)}$ is the identity matrix of order r; the coupling is scale-invariant if and only if the square matrix S = 0

We will consider two *associated* quantum graph Hamiltonians, H with the above vertex coupling, and H_0 where we replace S by zero

A result for this associated pair



Proposition ([E-Turek'17])

For the spectra $\sigma(H)$ and $\sigma(H_0)$ the following claims hold true:

- (i) If $\sigma(H_0)$ has an open gap, then $\sigma(H)$ has infinitely many gaps.
- (ii) If the edge lengths are rationally dependent, then the gaps of $\sigma(H)$ asymptotically coincide with those of $\sigma(H_0)$.

A result for this associated pair

Proposition ([E-Turek'17])

For the spectra $\sigma(H)$ and $\sigma(H_0)$ the following claims hold true:

- (i) If $\sigma(H_0)$ has an open gap, then $\sigma(H)$ has infinitely many gaps.
- (ii) If the edge lengths are rationally dependent, then the gaps of $\sigma(H)$ asymptotically coincide with those of $\sigma(H_0)$.

Proof idea: The argument is based on the following observation: the on-shell S-matrix for H

$$\mathcal{S}(k) = -I^{(n)} + 2 \begin{pmatrix} I^{(r)} \\ T^* \end{pmatrix} \left(I^{(r)} + TT^* - \frac{1}{ik}S \right)^{-1} \left(I^{(r)} - T \right)$$

Hence the scale-invariant part is, naturally, independent of k, and the Robin part is $O(k^{-1})$



A result for this associated pair

Proposition ([E-Turek'17])

For the spectra $\sigma(H)$ and $\sigma(H_0)$ the following claims hold true:

- (i) If $\sigma(H_0)$ has an open gap, then $\sigma(H)$ has infinitely many gaps.
- (ii) If the edge lengths are rationally dependent, then the gaps of $\sigma(H)$ asymptotically coincide with those of $\sigma(H_0)$.

Proof idea: The argument is based on the following observation: the on-shell S-matrix for H

$$S(k) = -I^{(n)} + 2 \begin{pmatrix} I^{(r)} \\ T^* \end{pmatrix} \left(I^{(r)} + TT^* - \frac{1}{ik}S \right)^{-1} \left(I^{(r)} T \right)$$

Hence the scale-invariant part is, naturally, independent of k, and the Robin part is $O(k^{-1})$

The same is true for S(k), and as consequence, the spectrum at high energies is mostly determined by the scale-invariant part. \Box

P.E.: Spectra of periodic graphs

DOGW 2019 Graz





We can give an affirmative answer to this question:

Theorem ([E-Turek'17])

Bethe-Sommerfeld graphs exist.



We can give an affirmative answer to this question:

Theorem ([E-Turek'17])

Bethe-Sommerfeld graphs exist.

As usual with existence claims, it is enough to demonstrate an example



We can give an affirmative answer to this question:

Theorem ([E-Turek'17])

Bethe-Sommerfeld graphs exist.

As usual with existence claims, it is enough to demonstrate an example. With this aim we are going to revisit the model of a *rectangular lattice graph* with δ -coupling introduced in [E'96, E-Gawlista'96]





Spectral condition



According to [E'96], a number $k^2 > 0$ belongs to a gap if and only if k > 0 satisfies the gap condition, which reads

$$\tan\left(\frac{ka}{2} - \frac{\pi}{2}\left\lfloor\frac{ka}{\pi}\right\rfloor\right) + \tan\left(\frac{kb}{2} - \frac{\pi}{2}\left\lfloor\frac{kb}{\pi}\right\rfloor\right) < \frac{\alpha}{2k} \quad \text{ for } \alpha > 0$$

and

$$\cot\left(\frac{ka}{2} - \frac{\pi}{2}\left\lfloor\frac{ka}{\pi}\right\rfloor\right) + \cot\left(\frac{kb}{2} - \frac{\pi}{2}\left\lfloor\frac{kb}{\pi}\right\rfloor\right) < \frac{|\alpha|}{2k} \quad \text{ for } \alpha < 0\,,$$

where we denote the edge lengths ℓ_j , j = 1, 2, as a, b; we neglect the Kirchhoff case, $\alpha = 0$, where $\sigma(H) = [0, \infty)$.

Spectral condition



According to [E'96], a number $k^2 > 0$ belongs to a gap if and only if k > 0 satisfies the gap condition, which reads

$$\tan\left(\frac{ka}{2} - \frac{\pi}{2}\left\lfloor\frac{ka}{\pi}\right\rfloor\right) + \tan\left(\frac{kb}{2} - \frac{\pi}{2}\left\lfloor\frac{kb}{\pi}\right\rfloor\right) < \frac{\alpha}{2k} \quad \text{ for } \alpha > 0$$

and

$$\cot\left(\frac{ka}{2} - \frac{\pi}{2}\left\lfloor\frac{ka}{\pi}\right\rfloor\right) + \cot\left(\frac{kb}{2} - \frac{\pi}{2}\left\lfloor\frac{kb}{\pi}\right\rfloor\right) < \frac{|\alpha|}{2k} \quad \text{ for } \alpha < 0\,,$$

where we denote the edge lengths ℓ_j , j = 1, 2, as a, b; we neglect the Kirchhoff case, $\alpha = 0$, where $\sigma(H) = [0, \infty)$.

Note that for $\alpha < 0$ the spectrum extends to the negative part of the real axis and may have a gap there, which is not important here because there is not more than a single negative gap, and this gap *always extends to positive values*



The spectrum depends on the ratio $\theta = \frac{\ell_1}{\ell_2}$. If θ is rational, $\sigma(H)$ has infinitely many gaps unless $\alpha = 0$ in which case $\sigma(H) = [0, \infty)$



The spectrum depends on the ratio $\theta = \frac{\ell_1}{\ell_2}$. If θ is rational, $\sigma(H)$ has infinitely many gaps unless $\alpha = 0$ in which case $\sigma(H) = [0, \infty)$

The same is true if θ is is an irrational well approximable by rationals, which means equivalently that in the continuous fraction representation $\theta = [a_0; a_1, a_2, ...]$ the sequence $\{a_j\}$ is unbounded



The spectrum depends on the ratio $\theta = \frac{\ell_1}{\ell_2}$. If θ is rational, $\sigma(H)$ has infinitely many gaps unless $\alpha = 0$ in which case $\sigma(H) = [0, \infty)$

The same is true if θ is is an irrational well approximable by rationals, which means equivalently that in the continuous fraction representation $\theta = [a_0; a_1, a_2, ...]$ the sequence $\{a_j\}$ is unbounded

On the other hand, $\theta \in \mathbb{R}$ is *badly approximable* if there is a c > 0 such that

$$\left|\theta-\frac{p}{q}\right|>\frac{c}{q^2}$$

for all $p, q \in \mathbb{Z}$ with $q \neq 0$



The spectrum depends on the ratio $\theta = \frac{\ell_1}{\ell_2}$. If θ is rational, $\sigma(H)$ has infinitely many gaps unless $\alpha = 0$ in which case $\sigma(H) = [0, \infty)$

The same is true if θ is is an irrational well approximable by rationals, which means equivalently that in the continuous fraction representation $\theta = [a_0; a_1, a_2, ...]$ the sequence $\{a_j\}$ is unbounded

On the other hand, $\theta \in \mathbb{R}$ is *badly approximable* if there is a c > 0 such that

$$\left| heta - rac{p}{q}
ight| > rac{c}{q^2}$$

for all $p, q \in \mathbb{Z}$ with $q \neq 0$. For such numbers we define the *Markov constant* by

$$\mu(heta):=\inf\left\{c>0 \; \left| \; \left(\exists_{\infty}(p,q)\in\mathbb{N}^2
ight)\left(\left| heta-rac{p}{q}
ight|<rac{c}{q^2}
ight)
ight\}
ight.$$



The spectrum depends on the ratio $\theta = \frac{\ell_1}{\ell_2}$. If θ is rational, $\sigma(H)$ has infinitely many gaps unless $\alpha = 0$ in which case $\sigma(H) = [0, \infty)$

The same is true if θ is is an irrational well approximable by rationals, which means equivalently that in the continuous fraction representation $\theta = [a_0; a_1, a_2, ...]$ the sequence $\{a_j\}$ is unbounded

On the other hand, $\theta \in \mathbb{R}$ is *badly approximable* if there is a c > 0 such that

$$\left| heta - rac{p}{q}
ight| > rac{c}{q^2}$$

for all $p, q \in \mathbb{Z}$ with $q \neq 0$. For such numbers we define the *Markov constant* by

$$\mu(heta):=\inf\left\{c>0 \; \left| \; \left(\exists_{\infty}(p,q)\in\mathbb{N}^2
ight)\left(\left| heta-rac{p}{q}
ight|<rac{c}{q^2}
ight)
ight\};
ight.$$

(we note that $\mu(\theta) = \mu(\theta^{-1})$)



The spectrum depends on the ratio $\theta = \frac{\ell_1}{\ell_2}$. If θ is rational, $\sigma(H)$ has infinitely many gaps unless $\alpha = 0$ in which case $\sigma(H) = [0, \infty)$

The same is true if θ is is an irrational well approximable by rationals, which means equivalently that in the continuous fraction representation $\theta = [a_0; a_1, a_2, ...]$ the sequence $\{a_j\}$ is unbounded

On the other hand, $\theta \in \mathbb{R}$ is *badly approximable* if there is a c > 0 such that

$$\left| heta - rac{p}{q}
ight| > rac{c}{q^2}$$

for all $p, q \in \mathbb{Z}$ with $q \neq 0$. For such numbers we define the *Markov constant* by

$$\mu(heta):=\inf\left\{c>0 \; \left| \; \left(\exists_{\infty}(p,q)\in\mathbb{N}^2
ight)\left(\left| heta-rac{p}{q}
ight|<rac{c}{q^2}
ight)
ight\};
ight.$$

(we note that $\mu(\theta) = \mu(\theta^{-1})$) and its 'one-sided analogues'

The golden mean situation



For example, consider the *golden mean*, $\phi = \frac{\sqrt{5}+1}{2} = [1; 1, 1, ...]$, which can be regarded as the 'worst' irrational

The golden mean situation



For example, consider the *golden mean*, $\phi = \frac{\sqrt{5}+1}{2} = [1; 1, 1, ...]$, which can be regarded as the 'worst' irrational

The answer is not a priori clear: let us plot the minima of the function appearing in the first gap condition, i.e. for $\alpha > 0$



The golden mean situation



For example, consider the *golden mean*, $\phi = \frac{\sqrt{5}+1}{2} = [1; 1, 1, ...]$, which can be regarded as the 'worst' irrational

The answer is not a priori clear: let us plot the minima of the function appearing in the first gap condition, i.e. for $\alpha > 0$



Note that they approach the limit values *from above*, also that the series open at $\frac{\pi^2}{\sqrt{5ab}}\phi^{\pm 1/2}|n^2 - m^2 - nm|, n, m \in \mathbb{N}$ [E-Gawlista'96]

But a closer look shows a more complex picture

Theorem ([E-Turek'17])

Let
$$\frac{a}{b} = \phi = \frac{\sqrt{5}+1}{2}$$
, then the following claims are valid:
(i) If $\alpha > \frac{\pi^2}{\sqrt{5}a}$ or $\alpha \le -\frac{\pi^2}{\sqrt{5}a}$, there are infinitely many spectral gaps.
(ii) If $-\frac{2\pi}{a} \tan\left(\frac{3-\sqrt{5}}{4}\pi\right) \le \alpha \le \frac{\pi^2}{\sqrt{5}a}$,

there are no gaps in the positive spectrum.

(iii) If $-\frac{\pi^2}{\sqrt{5}a} < \alpha < -\frac{2\pi}{a} \tan\left(\frac{3-\sqrt{5}}{4}\pi\right),$

there is a nonzero and finite number of gaps in the positive spectrum.

But a closer look shows a more complex picture

Theorem ([E-Turek'17])

Let
$$\frac{a}{b} = \phi = \frac{\sqrt{5}+1}{2}$$
, then the following claims are valid:
(i) If $\alpha > \frac{\pi^2}{\sqrt{5}a}$ or $\alpha \le -\frac{\pi^2}{\sqrt{5}a}$, there are infinitely many spectral gaps.
(ii) If $-\frac{2\pi}{a} \tan\left(\frac{3-\sqrt{5}}{4}\pi\right) \le \alpha \le \frac{\pi^2}{\sqrt{5}a}$,

there are no gaps in the positive spectrum.

(iii) If $-\frac{\pi^2}{\sqrt{5}a} < \alpha < -\frac{2\pi}{a} \tan\left(\frac{3-\sqrt{5}}{4}\pi\right),$

there is a nonzero and finite number of gaps in the positive spectrum.

Corollary

The above theorem about the existence of BS graphs is valid.

P.E.: Spectra of periodic graphs

DOGW 2019 Graz

More about this example

merfeld

The window in which the golden-mean lattice has the Bethe–Sommerfeld property is narrow, it is roughly $4.298 \leq -\alpha a \leq 4.414$.

More about this example

The window in which the golden-mean lattice has the Bethe–Sommerfeld property is narrow, it is roughly $4.298 \leq -\alpha a \leq 4.414$.

We are also able to control the number of gaps in the BS regime:

Theorem ([E-Turek'17])

For a given $N \in \mathbb{N}$, there are exactly N gaps in the positive spectrum if and only if α is chosen within the bounds

$$-\frac{2\pi \left(\phi^{2(N+1)}-\phi^{-2(N+1)}\right)}{\sqrt{5}a}\tan\left(\frac{\pi}{2}\phi^{-2(N+1)}\right) \le \alpha < -\frac{2\pi \left(\phi^{2N}-\phi^{-2N}\right)}{\sqrt{5}a}\tan\left(\frac{\pi}{2}\phi^{-2N}\right).$$

More about this example

The window in which the golden-mean lattice has the Bethe–Sommerfeld property is narrow, it is roughly $4.298 \leq -\alpha a \leq 4.414$.

We are also able to control the number of gaps in the BS regime:

Theorem ([E-Turek'17])

For a given $N \in \mathbb{N}$, there are exactly N gaps in the positive spectrum if and only if α is chosen within the bounds

$$-\frac{2\pi \left(\phi^{2(N+1)}-\phi^{-2(N+1)}\right)}{\sqrt{5}a}\tan\left(\frac{\pi}{2}\phi^{-2(N+1)}\right) \le \alpha < -\frac{2\pi \left(\phi^{2N}-\phi^{-2N}\right)}{\sqrt{5}a}\tan\left(\frac{\pi}{2}\phi^{-2N}\right).$$

Note that the numbers $A_j := \frac{2\pi \left(\phi^{2j} - \phi^{-2j}\right)}{\sqrt{5}} \tan\left(\frac{\pi}{2}\phi^{-2j}\right)$ form an increasing sequence the first element of which is $A_1 = 2\pi \tan\left(\frac{3-\sqrt{5}}{4}\pi\right)$ and $A_j < \frac{\pi^2}{\sqrt{5}}$ for all $j \in \mathbb{N}$.

More general result



Proofs of the above results are based on properties of Diophantine approximations. In a similar way one can prove

More general result



Proofs of the above results are based on properties of Diophantine approximations. In a similar way one can prove

- Theorem ([E-Turek'17])
- Let $\theta = \frac{a}{b}$ and define

$$\gamma_{+} := \min\left\{\inf_{m \in \mathbb{N}}\left\{\frac{2m\pi}{a}\tan\left(\frac{\pi}{2}(m\theta^{-1} - \lfloor m\theta^{-1} \rfloor)\right)\right\}, \inf_{m \in \mathbb{N}}\left\{\frac{2m\pi}{b}\tan\left(\frac{\pi}{2}(m\theta - \lfloor m\theta \rfloor)\right)\right\}\right\}$$

and γ_{-} similarly with $\lfloor \cdot \rfloor$ replaced by $\lceil \cdot \rceil$

More general result



Proofs of the above results are based on properties of Diophantine approximations. In a similar way one can prove

- Theorem ([E-Turek'17])
- Let $\theta = \frac{a}{b}$ and define

$$\gamma_{+} := \min\left\{\inf_{m \in \mathbb{N}}\left\{\frac{2m\pi}{a} \tan\left(\frac{\pi}{2}(m\theta^{-1} - \lfloor m\theta^{-1} \rfloor)\right)\right\}, \inf_{m \in \mathbb{N}}\left\{\frac{2m\pi}{b} \tan\left(\frac{\pi}{2}(m\theta - \lfloor m\theta \rfloor)\right)\right\}\right\}$$

and γ_{-} similarly with $\lfloor \cdot \rfloor$ replaced by $\lceil \cdot \rceil$. If the coupling constant α satisfies

$$\gamma_{\pm} < \pm \alpha < \frac{\pi^2}{\max\{a, b\}} \mu(\theta) \,,$$

then there is a nonzero and finite number of gaps in the positive spectrum.

Another application of periodic quantum graphs



Square lattice graphs were recently suggested a tool to model the *anomalous Hall effect*, cf. [Středa-Kučera'15], i.e. the situation when a Hall voltage appears *without the presence of an external magnetic field*

Another application of periodic quantum graphs



Square lattice graphs were recently suggested a tool to model the *anomalous Hall effect*, cf. [Středa-Kučera'15], i.e. the situation when a Hall voltage appears *without the presence of an external magnetic field*

The mechanism giving rise to the effect is not completely clear but it is believed that it comes from internal magnetization in combination with the spin-orbit interaction
Another application of periodic quantum graphs



Square lattice graphs were recently suggested a tool to model the *anomalous Hall effect*, cf. [Středa-Kučera'15], i.e. the situation when a Hall voltage appears *without the presence of an external magnetic field*

The mechanism giving rise to the effect is not completely clear but it is believed that it comes from internal magnetization in combination with the spin-orbit interaction

To mimick the rotational motion of atomic orbitals responsible for the magnetization, the authors had to impose 'by hand' the requirement that the electrons move only one way on the loops of the lattice

Another application of periodic quantum graphs



Square lattice graphs were recently suggested a tool to model the *anomalous Hall effect*, cf. [Středa-Kučera'15], i.e. the situation when a Hall voltage appears *without the presence of an external magnetic field*

The mechanism giving rise to the effect is not completely clear but it is believed that it comes from internal magnetization in combination with the spin-orbit interaction

To mimick the rotational motion of atomic orbitals responsible for the magnetization, the authors had to impose 'by hand' the requirement that the electrons move only one way on the loops of the lattice. Naturally, such an assumption *cannot be justified from the first principles*

Another application of periodic quantum graphs



Square lattice graphs were recently suggested a tool to model the *anomalous Hall effect*, cf. [Středa-Kučera'15], i.e. the situation when a Hall voltage appears *without the presence of an external magnetic field*

The mechanism giving rise to the effect is not completely clear but it is believed that it comes from internal magnetization in combination with the spin-orbit interaction

To mimick the rotational motion of atomic orbitals responsible for the magnetization, the authors had to impose 'by hand' the requirement that the electrons move only one way on the loops of the lattice. Naturally, such an assumption *cannot be justified from the first principles*

This motivated us to investigate situations where such an *inherent rotation* can take place, not at the graphs edges but in its *vertices*

In the vertex coupling conditions mentioned above,



$$(U-I)\Psi+i(U+I)\Psi'=0,$$

In the vertex coupling conditions mentioned above,

 $(U-I)\Psi+i(U+I)\Psi'=0\,,$

we choose the unitary matrix U of the form

$$U = \begin{pmatrix} 0 & 1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 1 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & 1 & \cdots & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & 0 & \cdots & 0 & 1 \\ 1 & 0 & 0 & 0 & \cdots & 0 & 0 \end{pmatrix};$$

the aim is to achieve 'maximum rotation' at a fixed energy, conventionally corresponding the momentum k=1



In the vertex coupling conditions mentioned above,

 $(U-I)\Psi+i(U+I)\Psi'=0,$

we choose the unitary matrix U of the form

$$U = \begin{pmatrix} 0 & 1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 1 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & 1 & \cdots & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & 0 & \cdots & 0 & 1 \\ 1 & 0 & 0 & 0 & \cdots & 0 & 0 \end{pmatrix};$$

the aim is to achieve 'maximum rotation' at a fixed energy, conventionally corresponding the momentum k = 1. Recall that one has U = S(1)





In the vertex coupling conditions mentioned above,

 $(U-I)\Psi+i(U+I)\Psi'=0,$

we choose the unitary matrix U of the form

$$U = \begin{pmatrix} 0 & 1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 1 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & 1 & \cdots & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & 0 & \cdots & 0 & 1 \\ 1 & 0 & 0 & 0 & \cdots & 0 & 0 \end{pmatrix};$$

the aim is to achieve 'maximum rotation' at a fixed energy, conventionally corresponding the momentum k = 1. Recall that one has U = S(1)Componentwise, with $\psi_j = \psi_j(0+)$ and $\psi'_i = \psi'_i(0+)$, we have

$$(\psi_{j+1}-\psi_j)+i(\psi_{j+1}'+\psi_j')=0\,,\quad j\in\mathbb{Z}\;(\mathrm{mod}\;\mathsf{N})\,,$$

which is non-trivial only for $N \ge 3$ and obviously non-invariant w.r.t. the reverse in the edge numbering order





Such a star-graph Hamiltonian H obviously has $\sigma_{ess}(H) = \mathbb{R}_+$



Such a star-graph Hamiltonian H obviously has $\sigma_{ess}(H) = \mathbb{R}_+$. Furthermore, it is easy to check that H has eigenvalues $-\kappa^2$, where

$$\kappa = an rac{\pi m}{N}$$

with *m* running through $1, \ldots, [\frac{N}{2}]$ for *N* odd and $1, \ldots, [\frac{N-1}{2}]$ for *N* even. Thus $\sigma_{\text{disc}}(H)$ is *always nonempty*



Such a star-graph Hamiltonian H obviously has $\sigma_{ess}(H) = \mathbb{R}_+$. Furthermore, it is easy to check that H has eigenvalues $-\kappa^2$, where

 $\kappa = \tan \frac{\pi m}{N}$

with *m* running through $1, \ldots, [\frac{N}{2}]$ for *N* odd and $1, \ldots, [\frac{N-1}{2}]$ for *N* even. Thus $\sigma_{\text{disc}}(H)$ is *always nonempty*, in particular, *H* has a single negative eigenvalue for N = 3, 4 which is equal to -1 and -3, respectively



Such a star-graph Hamiltonian H obviously has $\sigma_{ess}(H) = \mathbb{R}_+$. Furthermore, it is easy to check that H has eigenvalues $-\kappa^2$, where



with *m* running through $1, \ldots, [\frac{N}{2}]$ for *N* odd and $1, \ldots, [\frac{N-1}{2}]$ for *N* even. Thus $\sigma_{\text{disc}}(H)$ is *always nonempty*, in particular, *H* has a single negative eigenvalue for N = 3, 4 which is equal to -1 and -3, respectively

For any vertex coupling U the S-matrix at the momentum k is

$$S(k) = rac{k-1+(k+1)U}{k+1+(k-1)U};$$

recall that we used U = S(1) when constructing our coupling



Such a star-graph Hamiltonian H obviously has $\sigma_{ess}(H) = \mathbb{R}_+$. Furthermore, it is easy to check that H has eigenvalues $-\kappa^2$, where

$$\kappa = an rac{\pi m}{N}$$

with *m* running through $1, \ldots, [\frac{N}{2}]$ for *N* odd and $1, \ldots, [\frac{N-1}{2}]$ for *N* even. Thus $\sigma_{\text{disc}}(H)$ is *always nonempty*, in particular, *H* has a single negative eigenvalue for N = 3, 4 which is equal to -1 and -3, respectively

For any vertex coupling U the S-matrix at the momentum k is

$$S(k) = rac{k-1+(k+1)U}{k+1+(k-1)U};$$

recall that we used U = S(1) when constructing our coupling

It might seem that the transport becomes trivial at small and high energies, since $\lim_{k\to 0} S(k) = -I$ and $\lim_{k\to\infty} S(k) = I$



However, more caution is needed; the formal limits is false if $+1 \mbox{ or } -1$ are eigenvalues of U

However, more caution is needed; the formal limits is false if +1 or



-1 are eigenvalues of U. A counterexample is provided by *Kirchhoff* coupling where U has only ± 1 as its eigenvalues; the corresponding S-matrix is *k*-independent and *not* a multiple of the identity

However, more caution is needed; the formal limits is false if +1 or



-1 are eigenvalues of U. A counterexample is provided by *Kirchhoff* coupling where U has only ± 1 as its eigenvalues; the corresponding S-matrix is *k*-independent and *not* a multiple of the identity

Denoting $\eta := \frac{1-k}{1+k}$

However, more caution is needed; the formal limits is false if +1 or -1 are eigenvalues of U. A counterexample is provided by *Kirchhoff coupling* where U has only ± 1 as its eigenvalues; the corresponding S-matrix is *k*-independent and *not* a multiple of the identity

Denoting $\eta := \frac{1-k}{1+k}$ we get by a straightforward computation

$$S_{ij}(k) = rac{1-\eta^2}{1-\eta^N} \left\{ -\eta \, rac{1-\eta^{N-2}}{1-\eta^2} \, \delta_{ij} + (1-\delta_{ij}) \, \eta^{(j-i-1) (ext{mod } N)}
ight\}$$



However, more caution is needed; the formal limits is false if +1 or -1 are eigenvalues of U. A counterexample is provided by *Kirchhoff coupling* where U has only ± 1 as its eigenvalues; the corresponding S-matrix is *k*-independent and *not* a multiple of the identity

Denoting $\eta := \frac{1-k}{1+k}$ we get by a straightforward computation

$$\mathcal{S}_{ij}(k) = rac{1-\eta^2}{1-\eta^N} \left\{ -\eta \, rac{1-\eta^{N-2}}{1-\eta^2} \, \delta_{ij} + (1-\delta_{ij}) \, \eta^{(j-i-1)(ext{mod } N)}
ight\}$$

This suggests, in particular, that the high-energy behavior, $\eta \rightarrow -1-$, could be determined by the *parity* of the vertex degree N



However, more caution is needed; the formal limits is false if +1 or -1 are eigenvalues of U. A counterexample is provided by *Kirchhoff coupling* where U has only ± 1 as its eigenvalues; the corresponding S-matrix is *k*-independent and *not* a multiple of the identity

Denoting $\eta := \frac{1-k}{1+k}$ we get by a straightforward computation

$$\mathcal{S}_{ij}(k) = rac{1-\eta^2}{1-\eta^N} \left\{ -\eta \, rac{1-\eta^{N-2}}{1-\eta^2} \, \delta_{ij} + (1-\delta_{ij}) \, \eta^{(j-i-1)(ext{mod } N)}
ight\}$$

This suggests, in particular, that the high-energy behavior, $\eta \to -1-$, could be determined by the *parity* of the vertex degree *N*. Indeed, we see that $\lim_{k\to\infty} S(k) = I$ holds for N = 3 and more generally *for all odd N*



However, more caution is needed; the formal limits is false if +1 or -1 are eigenvalues of U. A counterexample is provided by *Kirchhoff coupling* where U has only ± 1 as its eigenvalues; the corresponding S-matrix is *k*-independent and *not* a multiple of the identity

Denoting $\eta := \frac{1-k}{1+k}$ we get by a straightforward computation

$$\mathcal{S}_{ij}(k) = rac{1-\eta^2}{1-\eta^N} \left\{ -\eta \, rac{1-\eta^{N-2}}{1-\eta^2} \, \delta_{ij} + (1-\delta_{ij}) \, \eta^{(j-i-1)(ext{mod } N)}
ight\}$$

This suggests, in particular, that the high-energy behavior, $\eta \to -1-$, could be determined by the *parity* of the vertex degree *N*. Indeed, we see that $\lim_{k\to\infty} S(k) = I$ holds for N = 3 and more generally *for all odd N* On the hand, for N = 4 we have

$$S(k) = rac{1}{1+\eta^2} \left(egin{array}{cccc} -\eta & 1 & \eta & \eta^2 \ \eta^2 & -\eta & 1 & \eta \ \eta & \eta^2 & -\eta & 1 \ 1 & \eta & \eta^2 & -\eta \end{array}
ight)$$

so the limit is not a multiple of identity



However, more caution is needed; the formal limits is false if +1 or -1 are eigenvalues of U. A counterexample is provided by *Kirchhoff coupling* where U has only ± 1 as its eigenvalues; the corresponding S-matrix is *k*-independent and *not* a multiple of the identity

Denoting $\eta := \frac{1-k}{1+k}$ we get by a straightforward computation

$$\mathcal{S}_{ij}(k) = rac{1-\eta^2}{1-\eta^N} \left\{ -\eta \, rac{1-\eta^{N-2}}{1-\eta^2} \, \delta_{ij} + (1-\delta_{ij}) \, \eta^{(j-i-1)(ext{mod } N)}
ight\}$$

This suggests, in particular, that the high-energy behavior, $\eta \to -1-$, could be determined by the *parity* of the vertex degree *N*. Indeed, we see that $\lim_{k\to\infty} S(k) = I$ holds for N = 3 and more generally *for all odd N* On the hand, for N = 4 we have

$$S(k) = rac{1}{1+\eta^2} \left(egin{array}{cccc} -\eta & 1 & \eta & \eta^2 \ \eta^2 & -\eta & 1 & \eta \ \eta & \eta^2 & -\eta & 1 \ 1 & \eta & \eta^2 & -\eta \end{array}
ight)$$

so the limit is not a multiple of identity; the same is true for any even N

















Spectral condition for the cases are easy to derive,

 $16i e^{i(\theta_1 + \theta_2)} k \sin k\ell [(k^2 - 1)(\cos \theta_1 + \cos \theta_2) + 2(k^2 + 1)\cos k\ell] = 0$





Spectral condition for the cases are easy to derive,

 $16i e^{i(\theta_1 + \theta_2)} k \sin k\ell [(k^2 - 1)(\cos \theta_1 + \cos \theta_2) + 2(k^2 + 1)\cos k\ell] = 0$

and

$$16i e^{-i(\theta_1+\theta_2} k^2 \sin k\ell \left(3+6k^2-k^4+4d_{\theta}(k^2-1)+(k^2+3)^2 \cos 2k\ell\right)=0,$$

where $d_{\theta} := \cos \theta_1 + \cos(\theta_1 - \theta_2) + \cos \theta_2$, respectively, where $\frac{1}{\ell}(\theta_1, \theta_2) \in [-\frac{\pi}{\ell}, \frac{\pi}{\ell}]^2$ is the quasimomentum





Spectral condition for the cases are easy to derive,

 $16i e^{i(\theta_1 + \theta_2)} k \sin k\ell [(k^2 - 1)(\cos \theta_1 + \cos \theta_2) + 2(k^2 + 1)\cos k\ell] = 0$

and

$$16i e^{-i(\theta_1+\theta_2} k^2 \sin k\ell \left(3+6k^2-k^4+4d_{\theta}(k^2-1)+(k^2+3)^2 \cos 2k\ell\right)=0,$$

where $d_{\theta} := \cos \theta_1 + \cos(\theta_1 - \theta_2) + \cos \theta_2$, respectively, where $\frac{1}{\ell}(\theta_1, \theta_2) \in [-\frac{\pi}{\ell}, \frac{\pi}{\ell}]^2$ is the quasimomentum, but tedious to solve except the *flat band cases*, $\sin k\ell = 0$

However, we can present the band solution in a graphical form

Picture worth of thousand words



For the two lattices, respectively, we get (with $\ell=rac{3}{2},$ dashed $\ell=rac{1}{4})$



Picture worth of thousand words



For the two lattices, respectively, we get (with $\ell=rac{3}{2},$ dashed $\ell=rac{1}{4})$



and



Some features are common:

• the number of open gaps is *always infinite*





- the number of open gaps is *always infinite*
- the gaps are centered around the flat bands except the lowest one



- the number of open gaps is *always infinite*
- the gaps are centered around the flat bands except the lowest one
- for some values of ℓ a band may *degenerate*

- the number of open gaps is *always infinite*
- the gaps are centered around the flat bands except the lowest one
- for some values of ℓ a band may *degenerate*
- the negative spectrum is *always nonempty*, the gaps become *exponentially narrow* around star graph eigenvalues as $\ell \to \infty$

- the number of open gaps is *always infinite*
- the gaps are centered around the flat bands except the lowest one
- for some values of ℓ a band may *degenerate*
- the negative spectrum is *always nonempty*, the gaps become *exponentially narrow* around star graph eigenvalues as $\ell \to \infty$
- But the high energy behavior of these lattices is substantially different:
 - the spectrum is dominated by *bands* for square lattices

Some features are common:

- the number of open gaps is *always infinite*
- the gaps are centered around the flat bands except the lowest one
- for some values of ℓ a band may *degenerate*
- the negative spectrum is *always nonempty*, the gaps become *exponentially narrow* around star graph eigenvalues as $\ell \to \infty$

But the *high energy behavior* of these lattices is *substantially different*:

- the spectrum is dominated by *bands* for square lattices
- it is dominated by *gaps* for hexagonal lattices

Some features are common:

- the number of open gaps is *always infinite*
- the gaps are centered around the flat bands except the lowest one
- for some values of ℓ a band may *degenerate*
- the negative spectrum is *always nonempty*, the gaps become *exponentially narrow* around star graph eigenvalues as $\ell \to \infty$

But the high energy behavior of these lattices is substantially different:

- the spectrum is dominated by *bands* for square lattices
- it is dominated by *gaps* for hexagonal lattices

Other interesting results can be found, say, concerning *interpolation* between the δ -coupling and the present one

Some features are common:

- the number of open gaps is *always infinite*
- the gaps are centered around the flat bands except the lowest one
- for some values of ℓ a band may *degenerate*
- the negative spectrum is *always nonempty*, the gaps become *exponentially narrow* around star graph eigenvalues as $\ell \to \infty$

But the high energy behavior of these lattices is substantially different:

- the spectrum is dominated by *bands* for square lattices
- it is dominated by gaps for hexagonal lattices

Other interesting results can be found, say, concerning *interpolation* between the δ -coupling and the present one. This is our next topic

More generally on vertex coupling symmetries

A symmetry is described by an invertible map in the space of boundar values, $\Theta : \mathbb{C}^n \to \mathbb{C}^n$. A vertex coupling is symmetric w.r.t Θ if the usual matching condition is equivalent to

 $(U-I)\Theta\Psi(0)+i(U+I)\Theta\Psi'(0)=0\,,$

or in other words, if U obeys $\Theta^{-1}U\Theta = U$
More generally on vertex coupling symmetries

A symmetry is described by an invertible map in the space of boundar values, $\Theta : \mathbb{C}^n \to \mathbb{C}^n$. A vertex coupling is symmetric w.r.t Θ if the usual matching condition is equivalent to

 $(U-I)\Theta\Psi(0)+i(U+I)\Theta\Psi'(0)=0\,,$

or in other words, if U obeys $\Theta^{-1}U\Theta = U$. Some common examples:

• *Mirror symmetric* couplings have the matching conditions invariant against $(\psi_1(0), \ldots, \psi_n(0)) \mapsto (\psi_n(0), \ldots, \psi_1(0))$ and the same for the derivatives; in other words, $\Theta = A$, the matrix with the entries equal to 1 on the main antidiagonal and zero otherwise

More generally on vertex coupling symmetries

A symmetry is described by an invertible map in the space of boundar values, $\Theta : \mathbb{C}^n \to \mathbb{C}^n$. A vertex coupling is symmetric w.r.t Θ if the usual matching condition is equivalent to

 $(U-I)\Theta\Psi(0)+i(U+I)\Theta\Psi'(0)=0\,,$

or in other words, if U obeys $\Theta^{-1}U\Theta = U$. Some common examples:

- Mirror symmetric couplings have the matching conditions invariant against $(\psi_1(0), \ldots, \psi_n(0)) \mapsto (\psi_n(0), \ldots, \psi_1(0))$ and the same for the derivatives; in other words, $\Theta = A$, the matrix with the entries equal to 1 on the main antidiagonal and zero otherwise
- The subset of *permutation-invariant* couplings is a two-parameter family, U = aI + bJ, where J denotes the matrix with all the entries equal to one; the parameters satisfy |a| = 1 and |a + nb| = 1

More generally on vertex coupling symmetries

A symmetry is described by an invertible map in the space of boundar values, $\Theta : \mathbb{C}^n \to \mathbb{C}^n$. A vertex coupling is symmetric w.r.t Θ if the usual matching condition is equivalent to

 $(U-I)\Theta\Psi(0)+i(U+I)\Theta\Psi'(0)=0\,,$

or in other words, if U obeys $\Theta^{-1}U\Theta = U$. Some common examples:

- Mirror symmetric couplings have the matching conditions invariant against $(\psi_1(0), \ldots, \psi_n(0)) \mapsto (\psi_n(0), \ldots, \psi_1(0))$ and the same for the derivatives; in other words, $\Theta = A$, the matrix with the entries equal to 1 on the main antidiagonal and zero otherwise
- The subset of *permutation-invariant* couplings is a two-parameter family, U = aI + bJ, where J denotes the matrix with all the entries equal to one; the parameters satisfy |a| = 1 and |a + nb| = 1
- Time-reversal-invariant couplings: in this case Θ is replaced by the antilinear operator of complex conjugation, and using relations $U^t \overline{U} = \overline{U}U^t = I$ we find easily that the matrix describing the coupling must be now invariant w.r.t. transposition, $U = U^t$

Symmetries, continued



Our focus here is on *rotationally symmetric* vertex coupling, i.e. those independent of cyclic permutations of the entries of $\Psi(0)$ and $\Psi'(0)$. They correspond to

$$\Theta = R := \begin{pmatrix} 0 & 1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 1 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & 1 & \cdots & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & 0 & \cdots & 0 & 1 \\ 1 & 0 & 0 & 0 & \cdots & 0 & 0 \end{pmatrix},$$

Symmetries, continued



Our focus here is on *rotationally symmetric* vertex coupling, i.e. those independent of cyclic permutations of the entries of $\Psi(0)$ and $\Psi'(0)$. They correspond to

Proposition

A rotationally symmetric vertex coupling is mirror symmetric if and only if it is time-reversal-invariant.

Symmetries, continued



Our focus here is on *rotationally symmetric* vertex coupling, i.e. those independent of cyclic permutations of the entries of $\Psi(0)$ and $\Psi'(0)$. They correspond to

$\Theta = R :=$	1	0	1	0	0	 0	0	\mathbf{Y}
		0	0	1	0	 0	0	
		0	0	0	1	 0	0	
		0	0	0	0	 0	1	
		1	0	0	0	 0	0	J

Proposition

A rotationally symmetric vertex coupling is mirror symmetric if and only if it is time-reversal-invariant.

Note also that while the notions of permutation-invariant and timereversal-invariant couplings are universal in the sense that they do *not* require embedding in an ambient space, the other two mentioned above make sense only if we think of the graph Γ as of *an embedded object*

Circulant matrices



Matrices satisfying $\Theta^{-1}U\Theta = U$ for the above $\Theta = R$ are *circulant matrices*, which generally take the form



being a particular case of Toeplitz matrices. The first row, i.e. the vector $c = (c_0, c_1, \ldots, c_{n-1})$, is called *generator* of C

Circulant matrices



Matrices satisfying $\Theta^{-1}U\Theta = U$ for the above $\Theta = R$ are *circulant matrices*, which generally take the form



being a particular case of Toeplitz matrices. The first row, i.e. the vector $c = (c_0, c_1, \ldots, c_{n-1})$, is called *generator* of C

Let us recall basic properties of such matrices. The vectors

$$\mathbf{v}_k = rac{1}{\sqrt{n}} \left(1, \omega^k, \omega^{2k}, \ldots, \omega^{(n-1)k}
ight)^T, \quad k = 0, 1, \ldots, n-1,$$

with $\omega := e^{2\pi i/n}$ are its normalized eigenvectors corresponding to

$$\lambda_k = c_0 + c_1 \omega^k + c_2 \omega^{2k} + \dots + c_{n-1} \omega^{(n-1)k}, \quad k = 0, 1, \dots, n-1.$$

Every circulant matrix C is diagonalized by the *Discrete Fourier Transform* matrix

$$F = \begin{pmatrix} 1 & 1 & 1 & 1 & \dots & 1 \\ 1 & \omega & \omega^2 & \omega^3 & \dots & \omega^{n-1} \\ 1 & \omega^2 & \omega^4 & \omega^6 & \dots & \omega^{2(n-1)} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & \omega^{n-1} & \omega^{2(n-1)} & \omega^{3(n-1)} & \dots & \omega^{(n-1)^2} \end{pmatrix}$$

,

Every circulant matrix C is diagonalized by the *Discrete Fourier Transform* matrix

$$F = \begin{pmatrix} 1 & 1 & 1 & 1 & \dots & 1 \\ 1 & \omega & \omega^2 & \omega^3 & \dots & \omega^{n-1} \\ 1 & \omega^2 & \omega^4 & \omega^6 & \dots & \omega^{2(n-1)} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & \omega^{n-1} & \omega^{2(n-1)} & \omega^{3(n-1)} & \dots & \omega^{(n-1)^2} \end{pmatrix}$$

in other words, $D = \frac{1}{n} F^* CF$ is a diagonal matrix with $\lambda_0, \lambda_1, \ldots, \lambda_{n-1}$ on the diagonal

,



Every circulant matrix C is diagonalized by the *Discrete Fourier Transform* matrix

$$F = \begin{pmatrix} 1 & 1 & 1 & 1 & \dots & 1 \\ 1 & \omega & \omega^2 & \omega^3 & \dots & \omega^{n-1} \\ 1 & \omega^2 & \omega^4 & \omega^6 & \dots & \omega^{2(n-1)} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & \omega^{n-1} & \omega^{2(n-1)} & \omega^{3(n-1)} & \dots & \omega^{(n-1)^2} \end{pmatrix}$$

in other words, $D = \frac{1}{n}F^*CF$ is a diagonal matrix with $\lambda_0, \lambda_1, \ldots, \lambda_{n-1}$ on the diagonal. Since $F^{-1} = \frac{1}{n}F^*$, we can express from this relation

$$c_j = \frac{1}{n} \left(\lambda_0 + \lambda_1 \omega^{-j} + \lambda_2 \omega^{-2j} + \dots + \lambda_{n-1} \omega^{-(n-1)j} \right)$$



Every circulant matrix C is diagonalized by the *Discrete Fourier Transform* matrix

$$F = \begin{pmatrix} 1 & 1 & 1 & 1 & \dots & 1 \\ 1 & \omega & \omega^2 & \omega^3 & \dots & \omega^{n-1} \\ 1 & \omega^2 & \omega^4 & \omega^6 & \dots & \omega^{2(n-1)} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & \omega^{n-1} & \omega^{2(n-1)} & \omega^{3(n-1)} & \dots & \omega^{(n-1)^2} \end{pmatrix}$$

in other words, $D = \frac{1}{n}F^*CF$ is a diagonal matrix with $\lambda_0, \lambda_1, \ldots, \lambda_{n-1}$ on the diagonal. Since $F^{-1} = \frac{1}{n}F^*$, we can express from this relation

$$c_j = \frac{1}{n} \left(\lambda_0 + \lambda_1 \omega^{-j} + \lambda_2 \omega^{-2j} + \dots + \lambda_{n-1} \omega^{-(n-1)j} \right)$$

A circulant matrix is unitary if and only if $|\lambda_j| = 1$ holds for all indices j = 0, 1, ..., n - 1. Consequently, circulant unitary matrices of order n are parametrized by an *n*-tuple of real numbers



Our aim is now to investigate a class of couplings interpolating between the 'maximally rotational' one discussed above and the usual δ coupling referring to

$$U=-I+\frac{2}{n+i\alpha}J\,,$$

where $\alpha \in \mathbb{R}$ is a parameter; the case $\alpha = 0$ is called *Kirchhoff coupling*

Our aim is now to investigate a class of couplings interpolating between the 'maximally rotational' one discussed above and the usual δ coupling referring to

$$U=-I+\frac{2}{n+i\alpha}J\,,$$

where $\alpha \in \mathbb{R}$ is a parameter; the case $\alpha = 0$ is called *Kirchhoff coupling* We seek a family of unitary matrices $\{U(t): t \in [0, 1]\}$ such that

$$U(0) = -I + \frac{2}{n+i\alpha}J \text{ and } U(1) = R;$$

the map $t \mapsto U(t)$ is *continuous* on $[0,1];$
 $U(t)$ is *unitary circulant* for all $t \in [0,1].$



Our aim is now to investigate a class of couplings interpolating between the 'maximally rotational' one discussed above and the usual δ coupling referring to

 $U = -I + \frac{2}{n+i\alpha}J,$

where
$$\alpha \in \mathbb{R}$$
 is a parameter; the case $\alpha = 0$ is called *Kirchhoff coupling*.
We seek a family of unitary matrices $\{U(t) : t \in [0, 1]\}$ such that

$$U(0) = -I + \frac{2}{n+i\alpha}J \text{ and } U(1) = R;$$

the map $t \mapsto U(t)$ is *continuous* on $[0,1];$
 $U(t)$ is *unitary circulant* for all $t \in [0,1].$

We will construct them using their eigenvalues. For the circulant matrix $U(1) \mbox{ we get}$

$$\lambda_k = \omega^k$$
 if $k = 0, 1, \dots, n-1$



Similarly, the eigenvalues of U(0) are

$$\lambda_k = -1 + \frac{2}{n+i\alpha} \sum_{j=0}^{n-1} \omega^{jk} = \begin{cases} \frac{n-i\alpha}{n+i\alpha} & \text{for } k = 0;\\ -1 & \text{for } k \ge 1. \end{cases}$$

For brevity, let us set $\frac{n-i\alpha}{n+i\alpha} = e^{-i\gamma}$; note that $\gamma \begin{cases} = 0 & \text{for } \alpha = 0; \\ \in (0,\pi) & \text{for } \alpha > 0; \\ \in (-\pi,0) & \text{for } \alpha < 0. \end{cases}$



Similarly, the eigenvalues of U(0) are

$$\lambda_k = -1 + \frac{2}{n+i\alpha} \sum_{j=0}^{n-1} \omega^{jk} = \begin{cases} \frac{n-i\alpha}{n+i\alpha} & \text{for } k = 0;\\ -1 & \text{for } k \ge 1. \end{cases}$$

For brevity, let us set $\frac{n-i\alpha}{n+i\alpha} = e^{-i\gamma}$; note that $\gamma \begin{cases} = 0 & \text{for } \alpha = 0; \\ \in (0,\pi) & \text{for } \alpha > 0; \\ \in (-\pi,0) & \text{for } \alpha < 0. \end{cases}$ Then are looking for a matrix with the eigenvalues

$$\lambda_k(t) = \begin{cases} e^{-i(1-t)\gamma} & \text{for } k = 0; \\ -e^{i\pi t \left(\frac{2k}{n} - 1\right)} & \text{for } k \ge 1 \end{cases}$$

for all $t \in [0,1]$ which would satisfy the stated requirements





Similarly, the eigenvalues of U(0) are

$$\lambda_k = -1 + \frac{2}{n+i\alpha} \sum_{j=0}^{n-1} \omega^{jk} = \begin{cases} \frac{n-i\alpha}{n+i\alpha} & \text{for } k = 0; \\ -1 & \text{for } k \ge 1. \end{cases}$$

For brevity, let us set $\frac{n-i\alpha}{n+i\alpha} = e^{-i\gamma}$; note that $\gamma \begin{cases} = 0 & \text{for } \alpha = 0; \\ \in (0,\pi) & \text{for } \alpha > 0; \\ \in (-\pi,0) & \text{for } \alpha < 0. \end{cases}$ Then are looking for a matrix with the eigenvalues

$$\lambda_k(t) = \begin{cases} e^{-i(1-t)\gamma} & \text{for } k = 0; \\ -e^{i\pi t \left(\frac{2k}{n} - 1\right)} & \text{for } k \ge 1 \end{cases}$$

for all $t \in [0,1]$ which would satisfy the stated requirements corresponding to

$$c_j(t) = \frac{1}{n} \left(e^{-i(1-t)\gamma} - \sum_{k=1}^{n-1} e^{i\pi t \left(\frac{2k}{n}-1\right)} \cdot \omega^{-kj} \right)$$



Spectrum of a star graph

Let Γ be star with *n* semi-infinite edges, then it is easy to check that the essential/continuous spectrum is $[0, \infty)$

Spectrum of a star graph

Let Γ be star with *n* semi-infinite edges, then it is easy to check that the essential/continuous spectrum is $[0, \infty)$. The negative spectrum is nonempty for any $t \in (0, 1]$ and $n \ge 3$. Indeed, writing $\psi_j(x) = b_j e^{-\kappa x}$, we get the spectral condition

 $\det[(U(t)-I)-i\kappa(U(t)+I)]=0\,,$

which is equivalent to $\kappa = -i \frac{\lambda_j(t) - 1}{\lambda_j(t) + 1}$ for some $0 \le j \le n - 1$



Spectrum of a star graph

Let Γ be star with *n* semi-infinite edges, then it is easy to check that the essential/continuous spectrum is $[0, \infty)$. The negative spectrum is nonempty for any $t \in (0, 1]$ and $n \ge 3$. Indeed, writing $\psi_j(x) = b_j e^{-\kappa x}$, we get the spectral condition

 $\det[(U(t)-I)-i\kappa(U(t)+I)]=0\,,$

which is equivalent to $\kappa = -i \frac{\lambda_j(t)-1}{\lambda_j(t)+1}$ for some $0 \le j \le n-1$. This yields

$$\begin{aligned} \kappa &= -\tan\frac{(1-t)\gamma}{2} \quad \text{for } \alpha < 0 \text{ and } t \neq 1 \\ \kappa &= -\cot\left(\frac{j}{n} - \frac{1}{2}\right)\pi t \quad \text{for } n \geq 3 \text{ and } j < \frac{n}{2} \end{aligned}$$

These solutions give rise to the eigenvalues $-\kappa^2 < 0$ of the star graph:

- there is a negative eigenvalue $-\tan^2 \frac{(1-t)\gamma}{2}$ whenever $\alpha < 0$;
- if $n \ge 3$, there is an additional $\lfloor \frac{n-1}{2} \rfloor$ -tuple for aech $t \in (0,1]$, namely $-\cot^2\left(\frac{j}{n}-\frac{1}{2}\right)\pi t$ with j running through $1,\ldots,\frac{n-1}{2}$ for n odd and $1,\ldots,\frac{n}{2}-1$ for n even

P.E.: Spectra of periodic graphs





Finally, look at what the eigenvalues do in the limits $t \rightarrow 0+ (\delta \text{ coupling})$



Finally, look at what the eigenvalues do in the limits $t \to 0+$ (δ coupling) and $t \to 1-$ (the 'extreme' rotational coupling):



Finally, look at what the eigenvalues do in the limits $t \to 0+$ (δ coupling) and $t \to 1-$ (the 'extreme' rotational coupling):

• If $t \to 0+$, all the eigenvalues $-\kappa^2$ diverge to $-\infty$ except for $-\tan^2 \frac{(1-t)\gamma}{2}$ occurring for $\alpha < 0$, which approaches the value $-\tan^2(\gamma/2) = -\alpha^2/n^2$



Finally, look at what the eigenvalues do in the limits $t \to 0+$ (δ coupling) and $t \to 1-$ (the 'extreme' rotational coupling):

• If $t \to 0+$, all the eigenvalues $-\kappa^2$ diverge to $-\infty$ except for $-\tan^2 \frac{(1-t)\gamma}{2}$ occurring for $\alpha < 0$, which approaches the value $-\tan^2(\gamma/2) = -\alpha^2/n^2$. When t = 0, the 'additional' eigenvalues thus disappear and the system has only one simple negative eigenvalue $-\alpha^2/n^2$ for $\alpha < 0$, while for $\alpha \ge 0$ its negative spectrum is empty



Finally, look at what the eigenvalues do in the limits $t \to 0+$ (δ coupling) and $t \to 1-$ (the 'extreme' rotational coupling):

- If $t \to 0+$, all the eigenvalues $-\kappa^2$ diverge to $-\infty$ except for $-\tan^2 \frac{(1-t)\gamma}{2}$ occurring for $\alpha < 0$, which approaches the value $-\tan^2(\gamma/2) = -\alpha^2/n^2$. When t = 0, the 'additional' eigenvalues thus disappear and the system has only one simple negative eigenvalue $-\alpha^2/n^2$ for $\alpha < 0$, while for $\alpha \ge 0$ its negative spectrum is empty
- If $t \to 1-$, the eigenvalues $-\kappa^2$ approach zero and $-\tan^2 \frac{j}{n}$, respectively



Finally, look at what the eigenvalues do in the limits $t \to 0+$ (δ coupling) and $t \to 1-$ (the 'extreme' rotational coupling):

- If $t \to 0+$, all the eigenvalues $-\kappa^2$ diverge to $-\infty$ except for $-\tan^2 \frac{(1-t)\gamma}{2}$ occurring for $\alpha < 0$, which approaches the value $-\tan^2(\gamma/2) = -\alpha^2/n^2$. When t = 0, the 'additional' eigenvalues thus disappear and the system has only one simple negative eigenvalue $-\alpha^2/n^2$ for $\alpha < 0$, while for $\alpha \ge 0$ its negative spectrum is empty
- If $t \to 1-$, the eigenvalues $-\kappa^2$ approach zero and $-\tan^2 \frac{j}{n}$, respectively. When t = 1, the only negative eigenvalues are $-\tan^2 \frac{j}{n}$, with j taking values $1, \ldots, \frac{n-1}{2}$ for n odd and $1, \ldots, \frac{n}{2} - 1$ for n even - as we have seen before

Scattering



Knowing U(t) we easily find the on-shell S-matrix. In particular, its eigenvalues are

$$\mu_j(t) = rac{k-1+(k+1)\lambda_j(t)}{k+1+(k-1)\lambda_j(t)}$$
 for $j = 0, 1, \dots, n-1$.

Scattering



Knowing U(t) we easily find the on-shell S-matrix. In particular, its eigenvalues are

$$\mu_j(t) = \frac{k - 1 + (k + 1)\lambda_j(t)}{k + 1 + (k - 1)\lambda_j(t)} \quad \text{for } j = 0, 1, \dots, n - 1.$$

We are again interested in the *high-energy behavior* of the S-matrix:

Scattering

Knowing U(t) we easily find the on-shell S-matrix. In particular, its eigenvalues are

$$\mu_j(t) = rac{k-1+(k+1)\lambda_j(t)}{k+1+(k-1)\lambda_j(t)} \quad ext{for } j = 0, 1, \dots, n-1.$$

We are again interested in the *high-energy behavior* of the S-matrix:

• If n is odd, then $\lim_{k\to\infty} \mu_j = 1$ for all $j = 0, 1, \dots, n-1$, hence

 $\lim_{k\to\infty}\mathcal{S}(k)=I$

• If *n* is even, then $\lim_{k\to\infty} \mu_j = 1$ for $j \neq \frac{n}{2}$, while $\lim_{k\to\infty} \mu_{n/2} = -1$, and consequently, the generator of $\lim_{k\to\infty} S(k)$ equals

$$\left(1-\frac{2}{n},\frac{2}{n},-\frac{2}{n},\frac{2}{n},\frac{2}{n},\ldots,-\frac{2}{n},\frac{2}{n}\right)$$

As in the 'extreme' rotational case, the S-matrix behaves at high energies differently for odd and even n



Square lattice

We consider again a lattice of spacing ℓ , now with the interpolating coupling. The treatment is similar to the particular case analyzed earlier; it yields the spectral condition

512 e<sup>*i*(
$$\theta_1 + \theta_2$$
)</sup> e^{-*i*(1-*t*)\gamma/2} [$V_3k^3 + V_2k^2 + V_1k + V_0$] = 0,



Square lattice

We consider again a lattice of spacing ℓ , now with the interpolating coupling. The treatment is similar to the particular case analyzed earlier; it yields the spectral condition

512 e<sup>*i*(
$$\theta_1 + \theta_2$$
)</sup> e^{-*i*($\frac{(1-t)\gamma}{2}$} [$V_3k^3 + V_2k^2 + V_1k + V_0$] = 0,

where

$$V_{3} = -\cos\frac{(1-t)\gamma}{2}\sin^{2}\frac{\pi t}{4}\sin k\ell(\cos\theta_{1} + \cos\theta_{2} + 2\cos k\ell);$$

$$V_{2} = 2\sin\frac{(1-t)\gamma}{2}\sin^{2}\frac{\pi t}{4}(\cos\theta_{1} + \cos k\ell)(\cos\theta_{2} + \cos k\ell);$$

$$V_{1} = \cos\frac{(1-t)\gamma}{2}\cos^{2}\frac{\pi t}{4}\sin k\ell(\cos\theta_{1} + \cos\theta_{2} - 2\cos k\ell);$$

$$V_{0} = -2\sin\frac{(1-t)\gamma}{2}\cos^{2}\frac{\pi t}{4}\sin^{2}k\ell.$$



Square lattice

We consider again a lattice of spacing ℓ , now with the interpolating coupling. The treatment is similar to the particular case analyzed earlier; it yields the spectral condition

512 e<sup>*i*(
$$\theta_1 + \theta_2$$
)</sup> e^{-*i*($\frac{(1-t)\gamma}{2}$} [$V_3k^3 + V_2k^2 + V_1k + V_0$] = 0,

where

$$V_{3} = -\cos\frac{(1-t)\gamma}{2}\sin^{2}\frac{\pi t}{4}\sin k\ell(\cos\theta_{1} + \cos\theta_{2} + 2\cos k\ell);$$

$$V_{2} = 2\sin\frac{(1-t)\gamma}{2}\sin^{2}\frac{\pi t}{4}(\cos\theta_{1} + \cos k\ell)(\cos\theta_{2} + \cos k\ell);$$

$$V_{1} = \cos\frac{(1-t)\gamma}{2}\cos^{2}\frac{\pi t}{4}\sin k\ell(\cos\theta_{1} + \cos\theta_{2} - 2\cos k\ell);$$

$$V_{0} = -2\sin\frac{(1-t)\gamma}{2}\cos^{2}\frac{\pi t}{4}\sin^{2}k\ell.$$

Hence k^2 belongs to the spectrum *iff* there are $\theta_1, \theta_2 \in [-\pi, \pi)$ such that $V_2k^3 + V_2k^2 + V_1k + V_0 = 0$.



The case $\alpha = 0$



If $\alpha = 0$ we have $V_2 = V_0 = 0$ and the spectral condition reduces to

$$\sin k\ell \left[\left(k^2 \sin^2 \frac{\pi t}{4} - \cos^2 \frac{\pi t}{4} \right) \left(\cos \theta_1 + \cos \theta_2 \right) - 2 \left(k^2 \sin^2 \frac{\pi t}{4} + \cos^2 \frac{\pi t}{4} \right) \cos k\ell \right] = 0.$$

The case $\alpha = 0$



If $\alpha = 0$ we have $V_2 = V_0 = 0$ and the spectral condition reduces to

$$\sin k\ell \left[\left(k^2 \sin^2 \frac{\pi t}{4} - \cos^2 \frac{\pi t}{4} \right) \left(\cos \theta_1 + \cos \theta_2 \right) - 2 \left(k^2 \sin^2 \frac{\pi t}{4} + \cos^2 \frac{\pi t}{4} \right) \cos k\ell \right] = 0.$$

It has two types of solutions. The first are infinitely degenerate eigenvalues, squares of

 $\frac{m\pi}{\ell} \quad \text{for } m \in \mathbb{N} \,.$

The case $\alpha = 0$



If $\alpha = 0$ we have $V_2 = V_0 = 0$ and the spectral condition reduces to

$$\sin k\ell \left[\left(k^2 \sin^2 \frac{\pi t}{4} - \cos^2 \frac{\pi t}{4} \right) \left(\cos \theta_1 + \cos \theta_2 \right) - 2 \left(k^2 \sin^2 \frac{\pi t}{4} + \cos^2 \frac{\pi t}{4} \right) \cos k\ell \right] = 0.$$

It has two types of solutions. The first are infinitely degenerate eigenvalues, squares of

 $\frac{m\pi}{\ell} \quad \text{for } m \in \mathbb{N} \,.$

The condition describing spectral bands can rewritten as

$$\left|k^2 \sin^2 \frac{\pi t}{4} - \cos^2 \frac{\pi t}{4}\right| \ge \left(k^2 \sin^2 \frac{\pi t}{4} + \cos^2 \frac{\pi t}{4}\right) \left|\cos k\ell\right|.$$

Note that if t = 0 (i.e., pure Kirchhoff), the condition simplifies to $|\cos k\ell| \le 1$, which is satisfied for all $k \ge 0$. Putting this trivial case aside, from now on we assume that $t \in (0, 1]$.


For $t \in (0, 1]$ the spectrum obviously contains infinitely many gaps located in the vicinity of $k = \frac{m\pi}{\ell}$ for $m \in \mathbb{N}$. The band condition for k > 0 can be rewritten as

$$\left(k\left|\tan\frac{k\ell}{2}\right| - \cot\frac{\pi t}{4}\right)\left(k\left|\cot\frac{k\ell}{2}\right| - \cot\frac{\pi t}{4}\right) \ge 0$$

and the zeros of the factors correspond to the band edges



For $t \in (0, 1]$ the spectrum obviously contains infinitely many gaps located in the vicinity of $k = \frac{m\pi}{\ell}$ for $m \in \mathbb{N}$. The band condition for k > 0 can be rewritten as

$$\left(k\left|\tan\frac{k\ell}{2}\right| - \cot\frac{\pi t}{4}\right)\left(k\left|\cot\frac{k\ell}{2}\right| - \cot\frac{\pi t}{4}\right) \ge 0$$

and the zeros of the factors correspond to the band edges. The latter intersect at points where $k \left| \tan \frac{k\ell}{2} \right| = k \left| \cot \frac{k\ell}{2} \right| = \cot \frac{\pi t}{4}$, i.e., at (t, k) such that

$$k = \left(m - \frac{1}{2}
ight)rac{\pi}{\ell} \quad ext{and} \quad t = rac{4}{\pi} ext{arccot} \left(m - rac{1}{2}
ight)rac{\pi}{\ell}\,, \quad m \in \mathbb{N}\,.$$

At those values of t the spectrum shrinks into a 'flat band'





Figure: Interpolation with the Kirchhoff coupling for $\ell = 1$, the spectrum is indicated by the shaded regions.

P.E.: Spectra of periodic graphs

DOGW 2019 Graz

The negative spectrum is found in a similar way

The negative spectrum is found in a similar way. The presence/absence of a gap above/below zero depends on t, the switch occurs at $t = \frac{4}{\pi} \arctan \frac{\ell}{2}$

The negative spectrum is found in a similar way. The presence/absence of a gap above/below zero depends on t, the switch occurs at $t = \frac{4}{\pi} \arctan \frac{\ell}{2}$

Let us look at the high-energy behavior of gaps. The condition reads

$$\left| \left(1 + \frac{2}{k^2} \cot^2 \frac{\pi t}{4} + \mathcal{O}(k^{-4}) \right) \cos k\ell \right| > 1 \quad \text{as} \quad k \to \infty$$

so it can be satisfied only for k located in small neighborhoods of $\frac{m\pi}{\ell}$. The approximate width of the *m*-th spectral gap is equal to

$$\frac{4}{m\pi}\cot\frac{\pi t}{4}+\mathcal{O}(m^{-2})$$

in the momentum variable, hence in energy the gaps are asymptotically constant, of the widths $\frac{8}{\ell} \cot \frac{\pi t}{4} + \mathcal{O}(m^{-1})$

The negative spectrum is found in a similar way. The presence/absence of a gap above/below zero depends on t, the switch occurs at $t = \frac{4}{\pi} \arctan \frac{\ell}{2}$

Let us look at the high-energy behavior of gaps. The condition reads

$$\left| \left(1 + \frac{2}{k^2} \cot^2 \frac{\pi t}{4} + \mathcal{O}(k^{-4}) \right) \cos k\ell \right| > 1 \quad \text{as} \quad k \to \infty$$

so it can be satisfied only for k located in small neighborhoods of $\frac{m\pi}{\ell}$. The approximate width of the *m*-th spectral gap is equal to

$$\frac{4}{m\pi}\cot\frac{\pi t}{4}+\mathcal{O}(m^{-2})$$

in the momentum variable, hence in energy the gaps are asymptotically constant, of the widths $\frac{8}{\ell} \cot \frac{\pi t}{4} + \mathcal{O}(m^{-1})$. Note that the gap width increases as t diminishes from this extreme value but eventually it starts to decrease again, to the point of vanishing at t = 0.

The analysis follows the same line but becomes more complicated; the spectral condition now yields spectra, as functions of t, in the form of a *union of pairs of regions*

P.E.: Spectra of periodic graphs

The analysis follows the same line but becomes more complicated; the spectral condition now yields spectra, as functions of t, in the form of a *union of pairs of regions*

Let us summarize our observations about the band spectra of our lattices:

(i) A 'discontinuity' at t = 0: There is always a spectral band which becomes narrow and strongly negative as $t \to 0$ and eventually disappears. This obviously corresponds to the behavior of the 'additional' eigenvalues of a single vertex



The analysis follows the same line but becomes more complicated; the spectral condition now yields spectra, as functions of t, in the form of a *union of pairs of regions*

Let us summarize our observations about the band spectra of our lattices:

- (i) A 'discontinuity' at t = 0: There is always a spectral band which becomes narrow and strongly negative as $t \to 0$ and eventually disappears. This obviously corresponds to the behavior of the 'additional' eigenvalues of a single vertex
- (ii) Point degeneracies for $\alpha = 0$: In the Kirchhoff case spectral bands may collapse to a point at particular values of t. It is not the case if $\alpha \neq 0$ where the spectral condition has other solutions which smear these Kirchhoff degenerate eigenvalues into bands of nonzero width, more pronounced as we are going farther from the Kirchhoff case



The analysis follows the same line but becomes more complicated; the spectral condition now yields spectra, as functions of t, in the form of a *union of pairs of regions*

Let us summarize our observations about the band spectra of our lattices:

- (i) A 'discontinuity' at t = 0: There is always a spectral band which becomes narrow and strongly negative as $t \to 0$ and eventually disappears. This obviously corresponds to the behavior of the 'additional' eigenvalues of a single vertex
- (ii) Point degeneracies for $\alpha = 0$: In the Kirchhoff case spectral bands may collapse to a point at particular values of t. It is not the case if $\alpha \neq 0$ where the spectral condition has other solutions which smear these Kirchhoff degenerate eigenvalues into bands of nonzero width, more pronounced as we are going farther from the Kirchhoff case
- (iii) Non-monotonicity of the gap widths: As mentioned already the widths of the gaps are not monotonous with respect to the interpolation parameter, the same is true if $\alpha \neq 0$

Illustration, weakly attractive interaction





Figure: Interpolation with an attractive δ coupling, $\alpha = -4(\sqrt{2}-1)$, $\ell = 1$.

Illustration, strongly attractive interaction





Figure: Interpolation with an attractive δ coupling, $\alpha = -4(\sqrt{2}+1)$, $\ell = 1$.

Other properties



(iv) α -independence of some bands: Some curves marking the band edges are independent of α . However, for $\alpha \neq 0$ the 'band edges' coincide only in parts of the interval [0, 1], as there is a neighborhood of $t = \frac{4}{\pi} \operatorname{arccot} \frac{3\pi}{2}$ in which there is an additional spectrum

Other properties



- (iv) α -independence of some bands: Some curves marking the band edges are independent of α . However, for $\alpha \neq 0$ the 'band edges' coincide only in parts of the interval [0, 1], as there is a neighborhood of $t = \frac{4}{\pi} \operatorname{arccot} \frac{3\pi}{2}$ in which there is an additional spectrum
- (v) 'Band edge' regularity: The curves delineating the band edges are described by analytic functions. In the Kirchhoff case the analyticity is violated only at the points when the curves are crossing, on the other hand, in the case $\alpha \neq 0$ where the spectrum is a union of bands there are other points where each particular edge is not smooth; needless to say, it remains Lipshitz

Other properties



- (iv) α -independence of some bands: Some curves marking the band edges are independent of α . However, for $\alpha \neq 0$ the 'band edges' coincide only in parts of the interval [0, 1], as there is a neighborhood of $t = \frac{4}{\pi} \operatorname{arccot} \frac{3\pi}{2}$ in which there is an additional spectrum
- (v) 'Band edge' regularity: The curves delineating the band edges are described by analytic functions. In the Kirchhoff case the analyticity is violated only at the points when the curves are crossing, on the other hand, in the case $\alpha \neq 0$ where the spectrum is a union of bands there are other points where each particular edge is not smooth; needless to say, it remains Lipshitz
- (vi) *Flat band spreading:* Infinitely degenerate eigenvalues for t = 1 may smear when the interpolation parameter decreases, but we know that they also remain in the spectrum. A possible explanation may come from the presence of different 'elementary' eigenfunctions in the case t = 1, namely 'Dirichlet' and 'Neumann' type, which could behave differently with respect to t

Illustration, larger lattice spacing





Figure: Interpolation with an attractive δ coupling, $\alpha = -4(\sqrt{2}+1)$ and $l = 2\pi$.

P.E.: Spectra of periodic graphs

DOGW 2019 Graz

Looking for extrema of the dispersion functions, people usually seek them and the border of the respective Brillouin zone

Looking for extrema of the dispersion functions, people usually seek them and the border of the respective Brillouin zone



As a warning, [Harrison-Kuchment-Sobolev-Winn'07] constructed example of a periodic quantum graph in which (some) band edges correspond to *internal points* of the Brillouin zone

Looking for extrema of the dispersion functions, people usually seek them and the border of the respective Brillouin zone



As a warning, [Harrison-Kuchment-Sobolev-Winn'07] constructed example of a periodic quantum graph in which (some) band edges correspond to *internal points* of the Brillouin zone

Subsequently, in [E-Kuchment-Winn'10] it was shown that same may be true even for *graphs periodic in one dimension*



The number of connecting edges had to be $N \ge 2$

Looking for extrema of the dispersion functions, people usually seek them and the border of the respective Brillouin zone



As a warning, [Harrison-Kuchment-Sobolev-Winn'07] constructed example of a periodic quantum graph in which (some) band edges correspond to *internal points* of the Brillouin zone

Subsequently, in [E-Kuchment-Winn'10] it was shown that same may be true even for *graphs periodic in one dimension*



The number of connecting edges had to be $N \ge 2$. An example:





In the same paper we showed that if $N \ge 2$, the band edges correspond to *periodic* and *antiperiodic* solutions



In the same paper we showed that if $N \ge 2$, the band edges correspond to *periodic* and *antiperiodic* solutions

However, we did it under that assumption that the system is *invariant w.r.t. time reversal*



In the same paper we showed that if $N \ge 2$, the band edges correspond to *periodic* and *antiperiodic* solutions

However, we did it under that assumption that the system is *invariant w.r.t. time reversal*. To show that this assumption was essential consider a *comb-shaped graph* with our non-invariant coupling at the vertices



In the same paper we showed that if $N \ge 2$, the band edges correspond to *periodic* and *antiperiodic* solutions

However, we did it under that assumption that the system is *invariant w.r.t. time reversal*. To show that this assumption was essential consider a *comb-shaped graph* with our non-invariant coupling at the vertices





In the same paper we showed that if $N \ge 2$, the band edges correspond to *periodic* and *antiperiodic* solutions

However, we did it under that assumption that the system is *invariant w.r.t. time reversal*. To show that this assumption was essential consider a *comb-shaped graph* with our non-invariant coupling at the vertices





In the same paper we showed that if $N \ge 2$, the band edges correspond to *periodic* and *antiperiodic* solutions

However, we did it under that assumption that the system is *invariant w.r.t. time reversal*. To show that this assumption was essential consider a *comb-shaped graph* with our non-invariant coupling at the vertices



Its analysis shows:

• two-sided comb is transport-friendly, bands dominate



In the same paper we showed that if $N \ge 2$, the band edges correspond to *periodic* and *antiperiodic* solutions

However, we did it under that assumption that the system is *invariant w.r.t. time reversal*. To show that this assumption was essential consider a *comb-shaped graph* with our non-invariant coupling at the vertices



Its analysis shows:

- two-sided comb is transport-friendly, bands dominate
- one-sided comb is transport-unfriendly, gaps dominate



In the same paper we showed that if $N \ge 2$, the band edges correspond to *periodic* and *antiperiodic* solutions

However, we did it under that assumption that the system is *invariant w.r.t. time reversal*. To show that this assumption was essential consider a *comb-shaped graph* with our non-invariant coupling at the vertices



Its analysis shows:

- two-sided comb is transport-friendly, bands dominate
- one-sided comb is transport-unfriendly, gaps dominate
- sending the one side edge lengths to zero in a two-sided comb does not yield one-sided comb transport



In the same paper we showed that if $N \ge 2$, the band edges correspond to *periodic* and *antiperiodic* solutions

However, we did it under that assumption that the system is *invariant w.r.t. time reversal*. To show that this assumption was essential consider a *comb-shaped graph* with our non-invariant coupling at the vertices



Its analysis shows:

- two-sided comb is transport-friendly, bands dominate
- one-sided comb is transport-unfriendly, gaps dominate
- sending the one side edge lengths to zero in a two-sided comb does not yield one-sided comb transport
- and what about the dispersion curves?

Two-sided comb: dispersion curves





The sources



The examples discussed in this talk come from

The sources



The examples discussed in this talk come from

[EV17] P.E., Daniel Vašata: Cantor spectra of magnetic chain graphs, *J. Phys. A: Math. Theor.* **50** (2017), 165201 (13pp)

[ET17a] P.E., Ondřej Turek: Quantum graphs with the Bethe-Sommerfeld property, *Nanosystems* **8** (2017), 305–309.

[ET17b] P.E., Ondřej Turek: Periodic quantum graphs from the Bethe-Sommerfeld point of view, J. Phys. A: Math. Theor. **50** (2017), 455201 (32pp)

[ET18] P.E., M.Tater: Quantum graphs with vertices of a preferred orientation, *Phys. Lett.* A382 (2018), 283–287.

[ETT18] P.E., O.Turek, M.Tater: A family of quantum graph vertex couplings interpolating between different symmetries, *J. Phys. A: Math. Theor.* **51** (2018), 285301 (22pp)

[EV19]~ P.E., Daniel Vašata: Spectral properties of $\mathbb Z$ periodic quantum chains without time reversal invariance, in preparation

The sources



The examples discussed in this talk come from

[EV17] P.E., Daniel Vašata: Cantor spectra of magnetic chain graphs, *J. Phys. A: Math. Theor.* **50** (2017), 165201 (13pp)

[ET17a] P.E., Ondřej Turek: Quantum graphs with the Bethe-Sommerfeld property, *Nanosystems* **8** (2017), 305–309.

[ET17b] P.E., Ondřej Turek: Periodic quantum graphs from the Bethe-Sommerfeld point of view, J. Phys. A: Math. Theor. **50** (2017), 455201 (32pp)

[ET18] P.E., M.Tater: Quantum graphs with vertices of a preferred orientation, *Phys. Lett.* A382 (2018), 283–287.

[ETT18] P.E., O.Turek, M.Tater: A family of quantum graph vertex couplings interpolating between different symmetries, *J. Phys. A: Math. Theor.* **51** (2018), 285301 (22pp)

[EV19] P.E., Daniel Vašata: Spectral properties of $\mathbb Z$ periodic quantum chains without time reversal invariance, in preparation

in combination the other papers mentioned in the course of the presentation.

It remains to say



It remains to say



Thank you for your attention!