Vertex coupling and spectra of periodic quantum graphs

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July 14, 2020

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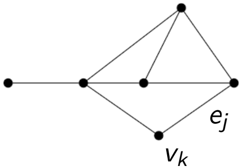

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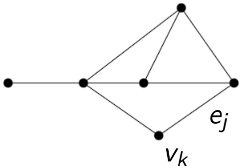

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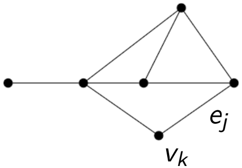

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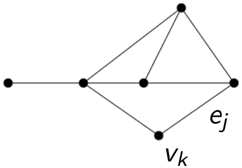

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In this talk we consider mostly the simplest case, $A = 0$ and $V = 0$, that is, we suppose that $H\psi = \{-\psi''\}$

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$$\psi_j(0) = \psi_k(0) =: \psi(0)\,,\; j,k = 1,\dots,n\,, \quad \sum_{j=1}^{n} \psi'_j(0) = \alpha\psi(0)$$

depending on a single parameter $\alpha \in \mathbb{R}$ which we call the *δ coupling*; the corresponding unitary matrix is $U = \frac{2}{n+i\alpha}\mathcal{J} - I$, where $\mathcal{J}$ is the $n \times n$ matrix whose all entries are equal to one.

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In particular, the case with $\alpha = 0$ is often called *Kirchhoff coupling.*

Quantum graph spectra

Spectral properties of quantum graph operators have been studied by many authors and a lot is known about them.

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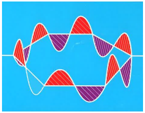
This is easily seen: a graph with a δ coupling which contains a *loop* with *rationally related edges* has the so-called *Dirichlet eigenvalues*



Courtesy: Peter Kuchment

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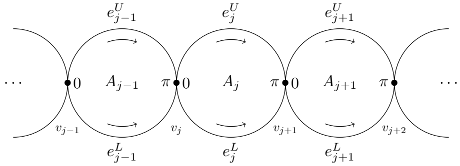
In fact, it can be even *pure point* as the following example of a *magnetic quantum graph* shows: we take a *loop array*



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where $\alpha \in \mathbb{R}$ is the coupling constant and $n = 4$ holds in our case

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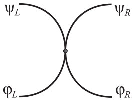

writing $\psi_L(x) = \mathrm{e}^{-iAx}(C_L^+\mathrm{e}^{ikx} + C_L^-\mathrm{e}^{-ikx})$ for $x \in [-\pi/2, 0]$ and energy $E := k^2 \neq 0$, and similarly for the other three components

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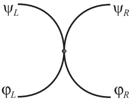

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with the discriminant $D = 4(\xi(k)^2 - 1)$, where $\xi(k) := \frac{\eta(k)}{4\cos A\pi}$ and

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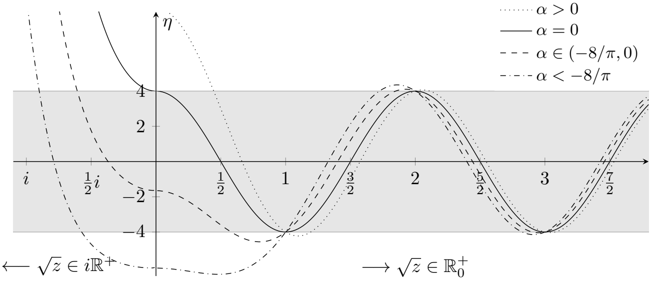
In the Kirchhoff case, $\alpha = 0$, the spectrum is 'trivial, $\sigma(H) = [0, \infty)$, provided $A \in \mathbb{Z}$, otherwise there are always *open spectral gaps* as one can see from a graphical solution of the above spectral condition

Determining the spectral bands



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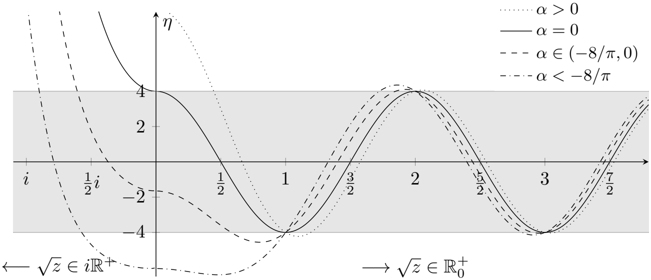

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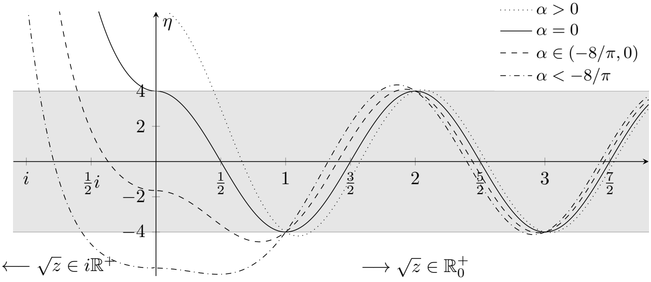

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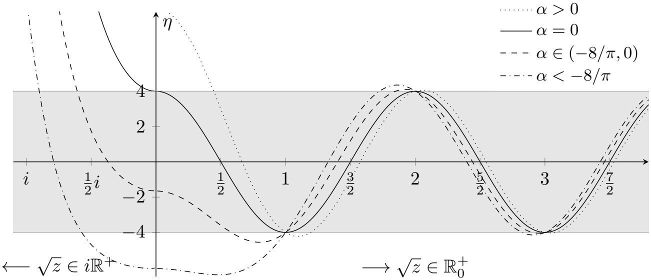

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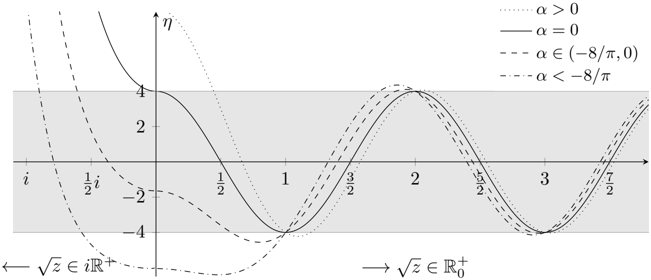

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Remark: There are other situations: for instance, if $A_j = \mu j + \theta$ with $\mu \in \mathbb{R} \setminus \mathbb{Q}$, the spectrum is a *Cantor set of Lebesgue measure zero*

P.E., D. Vašata: Cantor spectra of magnetic chain graphs, *J. Phys. A: Math. Theor. 50* (2017), 165201.

Questions to be addressed

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- is the *number of open gaps* finite or infinite?
- can the gap structure depend on the *graph topology?*

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The standard reference, [Berkolaiko-Kuchment'13, loc.cit.], says that Bethe-Sommerfeld heuristic reasoning is applicable again

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L. Parnovski: Bethe-Sommerfeld conjecture, *Ann. Henri Poincaré* **9** (2008), 457–508.

Question: How the situation looks for quantum graphs which can, in a sense, are 'mixing' different dimensionalities?

The standard reference, [Berkolaiko-Kuchment'13, loc.cit.], says that Bethe-Sommerfeld heuristic reasoning is applicable again, however, the finiteness of the gap number *is not a strict law*

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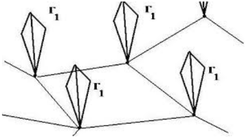

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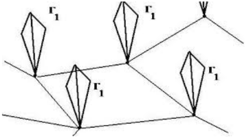

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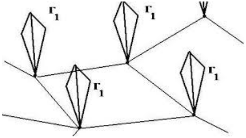

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Thus, instead of ‘not a strict law’, the question rather is whether *it is a ‘law’ at all*: do infinite periodic graphs having a *finite nonzero* number of open gaps exist? From obvious reasons we would call them *Bethe-Sommerfeld graphs*

The answer depends on the vertex coupling

Recall that self-adjointness requires the matching conditions $(U-I)\psi + i(U+I)\psi' = 0$, where ψ, ψ' are vectors of values and derivatives at the vertex of degree n and U is an $n \times n$ unitary matrix

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Worse than that, there is a simple argument showing in a 'typical' periodic graph the probability of being in a band or gap is $\neq 0, 1$.

R. Band, G. Berkolaiko: Universality of the momentum band density of periodic networks, *Phys. Rev. Lett.* **113** (2013), 130404.

The existence

Nevertheless, the answer to our question is affirmative:

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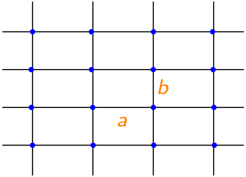
It is sufficient, of course, to demonstrate an example. With this aim we are going to revisit the model of a *rectangular lattice graph* with a δ *coupling* in the vertices introduced in

P.E.: Contact interactions on graph superlattices, *J. Phys. A: Math. Gen.* **29** (1996), 87–102.

P.E., R. Gawlista: Band spectra of rectangular graph superlattices, *Phys. Rev.* **B53** (1996), 7275–7286.



Spectral condition

A number $k^2 > 0$ belongs to a gap *iff* $k > 0$ satisfies the *gap condition* which is easily derived; it reads

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

and

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

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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*

What is known about this model

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

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Let us turn now to the *question about the gaps number*. We can answer it for any θ but for the purpose of this talk we limit ourself with the example of the *'worst' irrational*, $\theta = \frac{\sqrt{5}+1}{2} = [1; 1, 1, \dots]$.

The golden mean situation

Theorem

Let $\frac{a}{b} = \theta = \frac{\sqrt{5}+1}{2}$, *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*

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

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Corollary

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

More about this example

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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

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

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

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More details in [E-Turek, loc.cit.], for extension to 3D lattices see

O. Turek: Gaps in the spectrum of a cuboidal periodic lattices graph, *Rep. Math. Phys.* **83** (2019), 107–127.

A different vertex coupling class

As a motivation, let us ask about the *meaning of the vertex coupling*. There are different ways to answer this question:

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We will use it as an inspiration.

Modeling anomalous Hall effect

Recently a *quantum-graph model* of the AHE was proposed in which the material structure of the sample is described by lattice of *δ-coupled rings* (topologically equivalent to a *rectangular lattice*)

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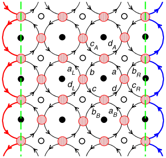

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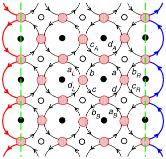

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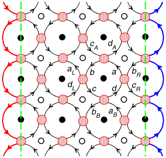

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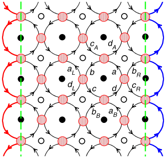

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There is a *flaw in the model*: to mimick the rotational motion of atomic orbitals responsible for the magnetization, the requirement was imposed 'by hand' that the electrons move only one way on the loops of the lattice. Naturally, this *cannot be justified from the first principles.*

Breaking the time-reversal invariance

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On the other hand, it *is* possible to break the time-reversal invariance, not at graph edges but in its *vertices*. Consider an example: note that for a vertex coupling U the *on-shell S-matrix* at the momentum k is

$$S(k) = \frac{k - 1 + (k+1)U}{k + 1 + (k-1)U},$$

in particular, we have $U = S(1)$

Breaking the time-reversal invariance

On the other hand, it *is* possible to break the time-reversal invariance, not at graph edges but in its *vertices*. Consider an example: note that for a vertex coupling U the *on-shell S-matrix* at the momentum k is

$$S(k) = \frac{k-1+(k+1)U}{k+1+(k-1)U}\,,$$

in particular, we have $U = S(1)$. If we thus require that the coupling leads to the *'maximum rotation'* at $k = 1$, it is natural to choose

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

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

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$$S_{ij}(k) = \frac{1-\eta^2}{1-\eta^N} \left\{ -\eta\, \frac{1-\eta^{N-2}}{1-\eta^2}\, \delta_{ij} + (1-\delta_{ij})\, \eta^{(j-i-1)(\mathrm{mod}\, N)} \right\}$$

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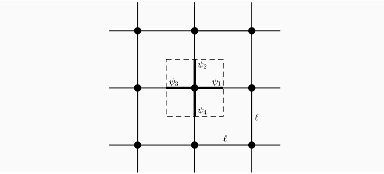
Let us look how this fact influences spectra of periodic quantum graphs.

Comparison of two lattices



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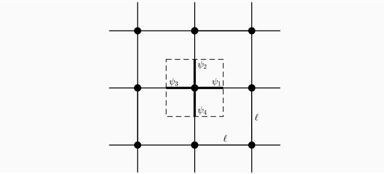

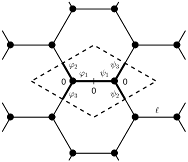

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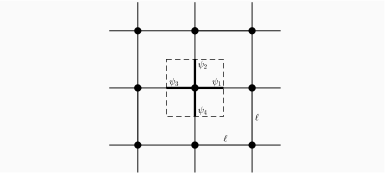

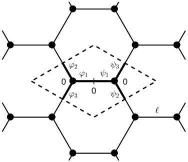

Spectral condition for the two cases are easy to derive,

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

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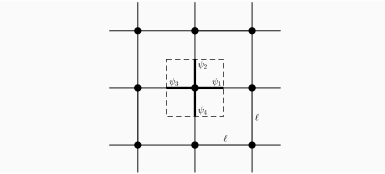

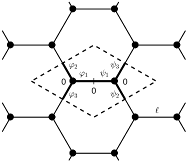

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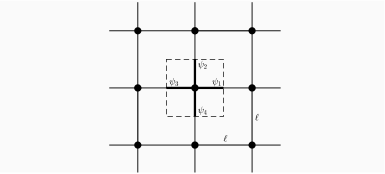

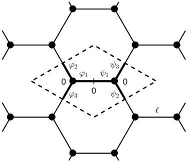

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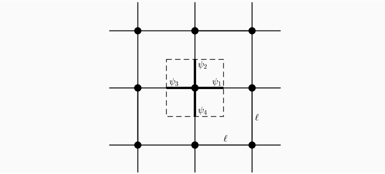

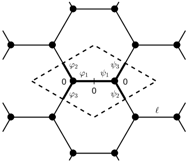

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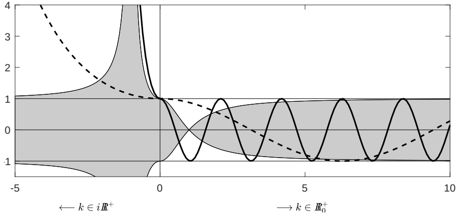
P.E., M. Tater: Quantum graphs with vertices of a preferred orientation, *Phys. Lett.* **A382** (2018), 283–287.

A picture is worth of thousand words

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



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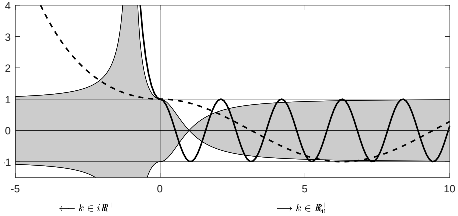

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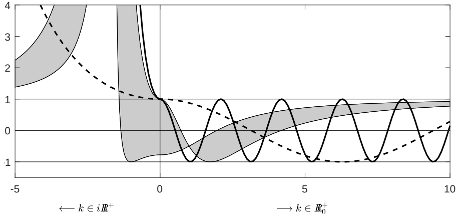

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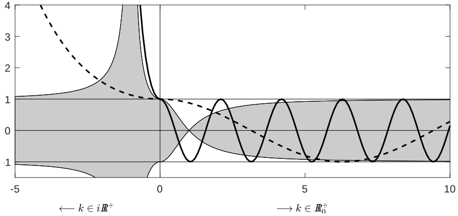

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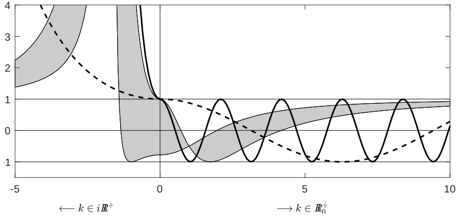

Comparison of the gap structure of the two lattices reveals the role of vertex degree parity clearly.

An interpolation

One can *interpolate* between the δ-coupling and the present one taking e.g., for U the *circulant matrix* with the eigenvalues

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

for all $t \in [0,1]$, where $\frac{n-i\alpha}{n+i\alpha} = \mathrm{e}^{-i\gamma}$

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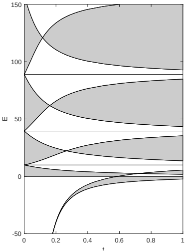

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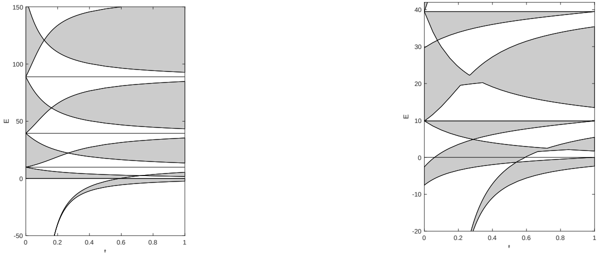

P.E., O. Turek, M. Tater: A family of quantum graph vertex couplings interpolating between different symmetries, *J. Phys. A: Math. Theor.* **51** (2018), 285301.

Discrete symmetry: Platonic solid graphs

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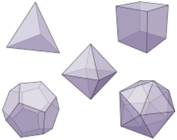

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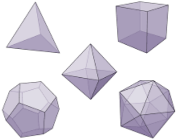

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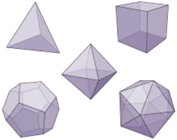

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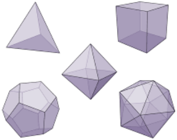

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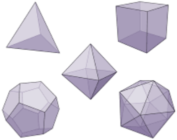

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and assume the described coupling in the vertices. The corresponding spectra are discrete but their *high-energy behavior differs:*

- for tetrahedron, cube, icosahedron, and dodecahedron the square roots of ev's *approach integer multiples of π* with an $\mathcal{O}(k^{-1})$ error
- *octahedron* also has such eigenvalues, but in addition it has *two other series:* those behaving as $k = 2\pi n \pm \frac{2}{3}\pi$ for $n \in \mathbb{Z}$, and as $k = \pi n + \frac{1}{2}\pi$ with with an $\mathcal{O}(k^{-2})$ error
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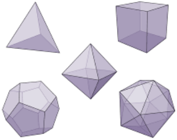
Discrete symmetry: Platonic solid graphs

Topological properties of our vertex coupling can be manifested in many other ways. Consider, e.g., finite equilateral graphs consisting of Platonic solids edges



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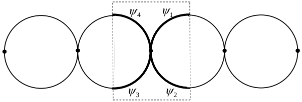
P.E., J. Lipovský: Spectral asymptotics of the Laplacian on Platonic solids graphs, *J. Math. Phys.* **60** (2019), 122101

Another periodic graph model

Let us look what this coupling influences graphs *periodic in one direction*

Another periodic graph model

Let us look what this coupling influences graphs *periodic in one direction*. Consider again a *loop chain*, first *tightly connected*



The spectrum of the corresponding Hamiltonian looks as follows:

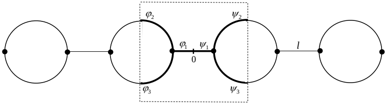
Theorem

The spectrum of H_0 consists of the absolutely continuous part which coincides with the interval $[0, \infty)$, and a family of infinitely degenerate eigenvalues, the isolated one equal to -1, and the embedded ones equal to the positive integers.

M. Baradaran, P.E., M. Tater: Ring chains with vertex coupling of a preferred orientation, *Rev. Math. Phys.*, to appear; arXiv:1912.03667

A loosely connected chain

Replace the direct coupling of adjacent rings by connecting segments of length $\ell > 0$, still with the same vertex coupling.



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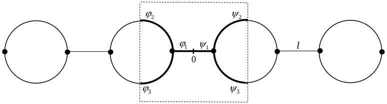

Theorem

The spectrum of H_ℓ has for any fixed $\ell > 0$ the following properties:

- *Any non-negative integer is an eigenvalue of infinite multiplicity.*

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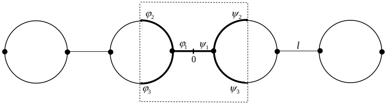

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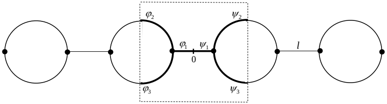

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- *Any non-negative integer is an eigenvalue of infinite multiplicity.*
- *Away of the non-negative integers the spectrum is absolutely continuous having a band-and-gap structure.*
- *The negative spectrum is contained in $(-\infty, -1)$ consisting of a single band if $\ell = \pi$, otherwise there is a pair of bands and $-3 \notin \sigma(H_\ell)$.*

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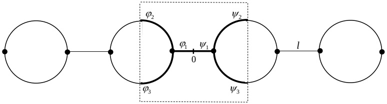

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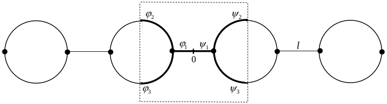

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- *The positive spectrum has infinitely many gaps.*
- $P_\sigma(H_\ell) := \lim_{K\to\infty} \frac{1}{K} |\sigma(H_\ell) \cap [0, K]| = 0$ *holds for any $\ell > 0$.*

The limit $\ell \to 0+$

The quantity $P_\sigma(H_\ell)$ in the last claim of the theorem is the *probability of being in the spectrum* introduced by

R. Band, G. Berkolaiko: Universality of the momentum band density of periodic networks, *Phys. Rev. Lett.* **113** (2013), 130404.

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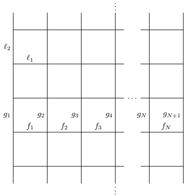
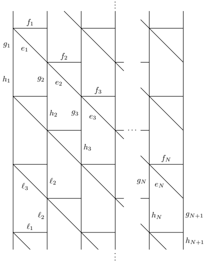
We have, however, obviously $P_\sigma(H_0) = 1$, hence our example shows that the said convergence may be *rather nonuniform!*

One more example: transport properties

Consider strips cut of the following two types of lattices:





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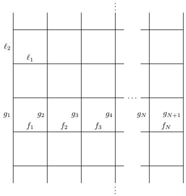

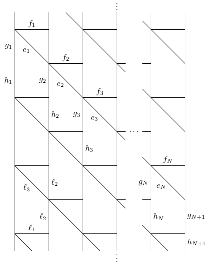

In both cases we impose the ‘rotating’ coupling at the vertices. By Floquet decomposition we are able reduce the task to investigation of a ‘one cell layer’. We use the Ansatz $a\mathrm{e}^{ikx} + b\mathrm{e}^{-ikx}$ for the wave functions e, f_j, g_j, h_j with the appropriate coefficients at the graphs edges

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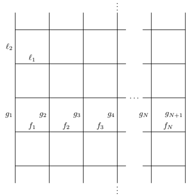

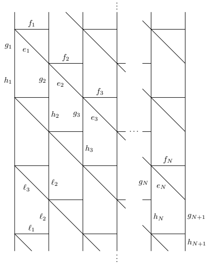

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This time we ask in which part of the 'guide' are the generalized eigenfunction *dominantly supported*

Transport properties, continued

Theorem

- *In the rectangular-lattice strip, for a fixed* $K \in \left(0, \frac{1}{2}\pi\right)$*, consider* $k > 0$ *obeying* $k \notin \bigcup_{n\in\mathbb{N}_0} \left(\frac{n\pi - K}{\ell_2}, \frac{n\pi + K}{\ell_2}\right)$*. With the natural normalization of the generalized eigenfunction corresponding to energy* k^2*, its components at the leftmost and rightmost vertical edges are of order* $\mathcal{O}(k^{-1})$ *as* $k \to \infty$*.*

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- *In the 'brick-lattice' strip, consider momenta* $k > 0$ *such that*

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  Adopting the same normalization as above and denoting by $q_j^{(m)}$ *with* $m = 1, \dots, 8$, *the coefficients of wave function components for the edges directed down and right from vertices of the* j*th vertical line, we have* $q_j^{(m)} = \mathcal{O}(k^{1-j})$ *as* $k \to \infty$.

P. Exner, J. Lipovský: Topological bulk-edge effects in quantum graph transport, *Phys. Lett.* **A384** (2020), 126390

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Remark: Note that the 'brick-lattice' strip is *not* a topological insulator!

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Thank you for your attention!