Vertex coupling effects in quantum graph spectra

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Vertex coupling in quantum graphs

No need, of course, to introduce it extensively in this community.

The boundary values being written as columns, $\Psi(0) := \{\psi_j(0)\}$ and $\Psi'(0) := \{\psi_j'(0)\}$, understood as left limits at the endpoint; then the most general self-adjoint matching conditions are of the form

$$A\Psi(0) + B\Psi'(0) = 0,$$

where the $n \times n$ matrices A, B satisfy the conditions

- $\mathrm{rank}\,(A, B) = n$
- AB^* is *Hermitean*

V. Kostrykin, R. Schrader: Kirhhoff's rule for quantum wires, *J. Phys. A: Math. Gen.* **32** (1999), 595–630.

F.S.Rofe-Beketov: Self-adjoint extensions of differential operators in a space of vector-valued functions, *Teor. Funkcii, Funkcional. Anal. Prilozh.* **8** (1969), 3–24 (in Russian).

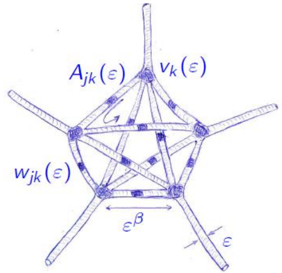
Naturally, these conditions are non-unique, as A, B can be replaced by CA, CB with a *regular* C. This non-uniqueness can be removed by using

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

where U is a *unitary $n \times n$ matrix*.

Meaning of the vertex coupling

We know, for instance, that *any* self-adjoint vertex coupling can by approximated by singular Schrödinger operators on a *Neumann networks*; the scheme looks as follows:



P.E., O. Post: A general approximation of quantum graph vertex couplings by scaled Schrödinger operators on thin branched manifolds, *Commun. Math. Phys.* **322** (2013), 207–227.

This might be a topic of a separate lecture, here my concern is different.

Such approximations have mostly existence meaning; from the pragmatic point it is reasonable to choose the coupling *ad hoc* to fit the physics of the problem. Some uncommon couplings may appear useful.

Why we should care about different couplings?

The answer to this question is: from the simple reason – because they describe a *different physics*. We will encounter various manifestation of this fact but let us illustrate the claim on the example of star graph of n edges, denoting its different Hamiltonians as H_U.

One of them is H_{D} corresponding to $U = -I$, in other words, each edge component of H_U is a halfline Laplacian with *Dirichlet* boundary condition, $\psi_j(0) = 0$. The spectrum of these operators is easily found, it implies that $\sigma(H_{\mathrm{D}}) = \mathbb{R}_+$ of multiplicity n.

For any U we have $\sigma_{\mathrm{ess}}(H_U) = \mathbb{R}_+$, because $(H_U - z)^{-1} - (H_{\mathrm{D}} - z)^{-1}$ is an operator of *finite rank* (equal to n) but in addition, there may be *negative eigenvalues*.

Their number coincides with the number of eigenvalues of U *in the open upper complex halfplane*. Indeed, the matching condition can diagonalized, and on the appropriate subspaces of $\bigoplus_{j=1}^n L^2(\mathbb{R}_+)$ we get n *Robin problems*, $\phi_j'(0) + \tan\frac{\alpha_j}{2}\phi_j(0) = 0$ for the eigenvalue $\mathrm{e}^{i\alpha_j}$ of U.

Common examples of vertex coupling

- Denote by $\mathcal{J}$ the $n \times n$ matrix whose all entries are equal to one; then $U = \frac{2}{n+i\alpha}\mathcal{J} - I$ corresponds to the so-called *δ coupling*,

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

with 'coupling strength' $\alpha \in \mathbb{R}$; $\alpha = \infty$ gives the Dirichlet $U = -I$

- On the other hand, $\alpha = 0$ gives *Kirchhoff condition* mentioned above.
- Similarly, $U = I - \frac{2}{n-i\beta}\mathcal{J}$ describes the *δ_{s}' coupling*,

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

with $\beta \in \mathbb{R}$. For $\beta = \infty$ we get the *Neumann* decoupling; the case $\beta = 0$ is sometimes referred to as *anti-Kirchhoff condition*.

- Another generalization of the 1D δ' interaction is the *δ' coupling*:

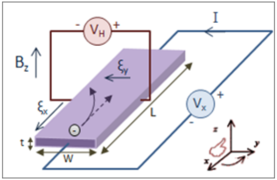
$$\sum_{j=1}^{n} \psi_j'(0) = 0, \quad \psi_j(0) - \psi_k(0) = \frac{\beta}{n}(\psi_j'(0) - \psi_k'(0)),\; 1 \le j,k \le n$$

with $U = \frac{n-i\alpha}{n+i\alpha} I - \frac{2}{n+i\alpha}\mathcal{J}$ and Neumann edge decoupling for $\beta = \infty$.

- But there many other couplings, and – as indicated above – one can choose a suitable one which would fit the physics of the problem.

Hall effect

To motivate our problem, let us recall one the most interesting and important problems in solid-state physics, the *Hall effect*,



Source: Wikipedia

in which magnetic field induces a *voltage perpendicular* to the current.

In the *quantum regime* the corresponding conductivity is *quantized* with a great precision – this fact lead already to two Nobel Prizes.

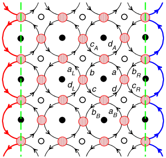
However, in ferromagnetic material one can observe a similar behavior also in the *absence of external magnetic field* – being labeled *anomalous*.

In contrast to the 'usual' quantum Hall effect, its mechanism is not well understood; it is conjectured that it comes from *internal magnetization* in combination with the *spin-orbit interaction*.

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 the *square lattice* we will discuss later)

P. Středa, J. Kučera: Orbital momentum and topological phase transformation, *Phys. Rev.* **B92** (2015), 235152.



Source: the cited paper

Looking at the picture we recognize a *flaw in the model*: 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!*

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

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

Writing the coupling componentwise for vertex of degree N, we have

$$(\psi_{j+1} - \psi_j) + i(\psi'_{j+1} + \psi'_j) = 0\,, \quad j \in \mathbb{Z} \pmod N\,,$$

which is non-trivial for $N \geq 3$ and obviously non-invariant w.r.t. the reverse in the edge numbering order, or equivalently, w.r.t. the complex conjugation representing the *time reversal.*

Star graphs: spectrum and scattering

Consider first a *star graph* with N semi-infinite edges and the above coupling. Obviously, we have $\sigma_{\mathrm{ess}}(H) = \mathbb{R}_+$. It is also easy to check that H has eigenvalues $-\kappa^2$, where

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

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

As for the scattering, we know that $S(k) = \frac{k-1+(k+1)U}{k+1+(k-1)U}$. It might seem that transport becomes trivial at small and high energies, since it looks like we have $\lim_{k\to 0} S(k) = -I$ and $\lim_{k\to\infty} S(k) = I$.

However, caution is needed; the formal limits lead to a *false result* if $+1$ or -1 are eigenvalues of U. A *counterexample* is the (scale invariant) Kirchhoff coupling where U has only ± 1 as its eigenvalues; the on-shell S-matrix is then independent of k and it is *not* a multiple of the identity.

The vertex parity enters the game

Denoting for simplicity $\eta := \frac{1-k}{1+k}$, a straightforward computation gives

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

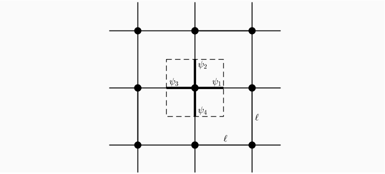
in particular, for $N = 3, 4$, respectively, we get

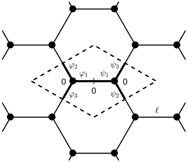
$$\frac{1+\eta}{1+\eta+\eta^2} \begin{pmatrix} -\frac{\eta}{1+\eta} & 1 & \eta \\ \eta & -\frac{\eta}{1+\eta} & 1 \\ 1 & \eta & -\frac{\eta}{1+\eta} \end{pmatrix} \quad \text{and} \quad \frac{1}{1+\eta^2} \begin{pmatrix} -\eta & 1 & \eta & \eta^2 \\ \eta^2 & -\eta & 1 & \eta \\ \eta & \eta^2 & -\eta & 1 \\ 1 & \eta & \eta^2 & -\eta \end{pmatrix}$$

We see that $\lim_{k\to\infty} S(k) = I$ holds for $N = 3$ and more generally *for all odd N*, while for the *even ones* the limit is *not a multiple of identity*. This is is related to the fact that in the latter case U has both ± 1 as its eigenvalues, while for N *odd* -1 is *missing*.

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

Comparison of two lattices





Spectral condition for the two cases are easy to derive,

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

and respectively

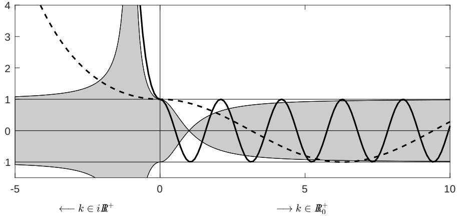
$$16i\,\mathrm{e}^{-i(\theta_1+\theta_2)}\,k^2\sin k\ell\left(3+6k^2-k^4+4d_\theta(k^2-1)+(k^2+3)^2\cos 2k\ell\right)=0\,,$$

where $d_\theta := \cos\theta_1+\cos(\theta_1-\theta_2)+\cos\theta_2$ and $\frac{1}{\ell}(\theta_1,\theta_2)\in[-\frac{\pi}{\ell},\frac{\pi}{\ell}]^2$ is the quasimomentum. They are tedious to solve except the *flat band cases*, $\sin k\ell=0$, however, we can present the band solution in a *graphical form*

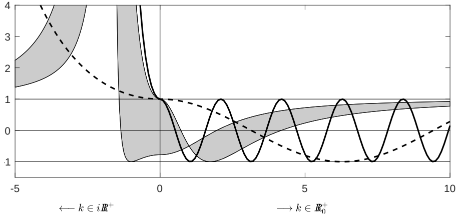
P.E., M. Tater: Quantum graphs with vertices of a preferred orientation, *Phys. Lett.* **A382** (2018), 283–287.

A picture is worth of thousand words

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



and



Comparison summary

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

Naturally, this is not the only way to break the time symmetry. A simple modification is to change the inherent *length scale* replacing the above matching condition by $(\psi_{j+1} - \psi_j) + i\ell(\psi'_{j+1} + \psi'_j) = 0$ for some $\ell > 0$. This does not matter for stars, of course, but it already *does* for lattices.

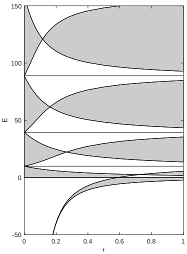
Let us mention one more involved choice of the vertex coupling.

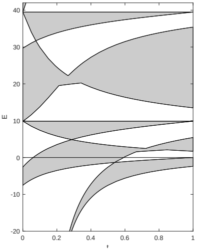
An interpolation

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 $\frac{n-i\alpha}{n+i\alpha} = \mathrm{e}^{-i\gamma}$. Taking, for instance, $\alpha = 0$ and $-4(\sqrt{2}+1)$, respectively, we have the following spectral patterns





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.

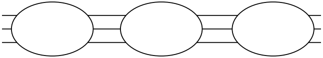
Another topic: band edges positions

Looking for extrema of the dispersion functions, people usually seek them at the border of the respective Brillouin zone. Quantum graphs provide a *warning*: there are examples of a periodic graph in which (some) band edges correspond to *internal points* of the Brillouin zone

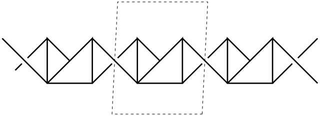
J.M. Harrison, P. Kuchment, A. Sobolev, B. Winn: On occurrence of spectral edges for periodic operators inside the Brillouin zone, *J. Phys. A: Math. Theor.* **40** (2007), 7597–7618.

P.E., P. Kuchment, B. Winn: On the location of spectral edges in $\mathbb{Z}$-periodic media, *J. Phys. A: Math. Theor.* **43** (2010), 474022.

The second one shows that this may be true even for *graphs periodic in one direction*



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



Band edges, continued

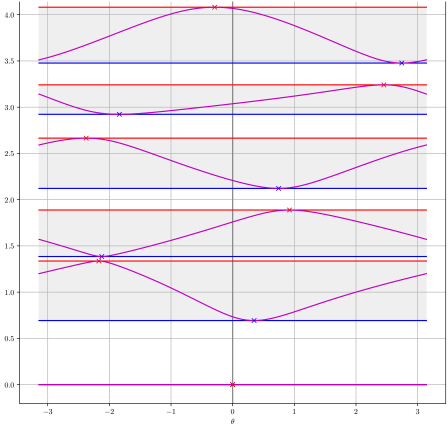
In the same paper we showed that if $N = 1$, the band edges correspond to *periodic* and *antiperiodic* solutions

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 we get the one-sided comb transport but the limit is *non-uniform*
- and what about the dispersion curves?

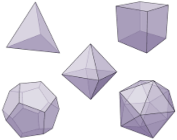
Two-sided comb: dispersion curves



P.E., Daniel Vašata: Spectral properties of $\mathbb{Z}$ periodic quantum chains without time reversal invariance, *in preparation*

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



Source: Wikipedia Commons

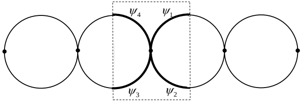
and assume the described coupling in the vertices. The corresponding spectra are discrete but their *high-energy behavior differs:*

- 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 an $\mathcal{O}(k^{-2})$ error
- no such distinction exists for more common couplings such as δ

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*. Consider again a *loop chain*, first *tightly connected*



The spectrum of the corresponding Hamiltonian looks as follows:

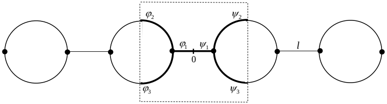
Theorem

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.* **33** (2021), 2060005.

A loosely connected chain

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



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.*
- *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 $-3 \notin \sigma(H_\ell)$.*
- *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*, which was introduced in

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

Having in mind the role of the vertex parity, one naturally asks what happens if the the connecting links lengths *shrink to zero*. From the general result derived in

G. Berkolaiko, Y. Latushkin, S. Sukhtaiev: Limits of quantum graph operators with shrinking edges, *Adv. Math.* **352** (2019), 632–669.

we know that $\sigma(H_\ell) \to \sigma(H_0)$ *in the set sense* as $\ell \to 0+$.

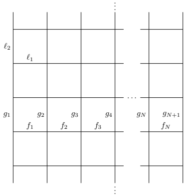
We have, however, obviously $P_\sigma(H_0) = 1$, hence our example shows that the said convergence may be *rather nonuniform!*

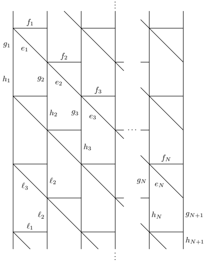
Note also that if we violate the mirror symmetry of the chain, we have instead $P_\sigma(H_0) = \frac{1}{2}$ independently of where exactly we place the vertex.

M. Baradaran, P.E., M. Tater: Spectrum of periodic chain graphs with time-reversal non-invariant vertex coupling, arXiv:2012.14344.

One more example: transport properties

Consider strips cut of the following two types of lattices:





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

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

$$k \notin \bigcup_{n\in\mathbb{N}_0} \left(\frac{n\pi - K}{\ell_1}, \frac{n\pi + K}{\ell_1}\right) \cup \bigcup_{n\in\mathbb{N}_0} \left(\frac{n\pi - K}{\ell_2}, \frac{n\pi + K}{\ell_2}\right) \cup \bigcup_{n\in\mathbb{N}_0} \left(\frac{n\pi - K}{\ell_3}, \frac{n\pi + K}{\ell_3}\right).$$

  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

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

$\mathcal{PT}$-symmetry

Having two research areas, each based of a strong concept, it is natural to look for connecting links. This applies, in particular, to quantum graphs and *$\mathcal{PT}$-symmetry*, also intensely studied in the last three decades.

C.M. Bender, S. Boettcher: Real spectra in non-Hermitian Hamiltonians having $\mathcal{PT}$-symmetry, *Phys. Rev. Lett.* **80** (1988), 5243–5246.

C.M. Bender: $\mathcal{PT}$-symmetric quantum theory, *J. Phys.: Conf. Ser.* **631** (2015), 012002.

It started from the observation that Schrödinger operators with complex potentials can have a real spectrum, and while the importance of this fact for QM remains a matter of dispute for those who are not *$\mathcal{PT}$-proselytes*, the idea found a number of applications in various areas.

The focus is, of course, on *nontrivial situations* when neither parity nor the time-reversal invariance were preserved but their composition was. The known examples of $\mathcal{PT}$-symmetry in quantum graphs go beyond the class of self-adjoint Hamiltonians.

A. Hussein, D. Krejčiřík, P. Siegl: Non-selfadjoint quantum graphs, *Trans. Amer. Math. Soc.* **367** (2015), 2921–2957.

P. Kurasov, B. Majidzadeh Garjani: Quantum graphs: $\mathcal{PT}$-symmetry and reflection symmetry of the spectrum, *J. Math. Phys.* **58** (2017), 023506.

D.U. Matrasulov, K.K.Sabirov, J.R. Yusupov: $\mathcal{PT}$-symmetric quantum graphs, *J. Phys. A: Math. Theor.* **52** (2019), 155302.

Vertex coupling symmetries

In our example we worked with a coupling which was obviously *time-reversal asymmetric*. Let us now adopt a more general point of view.

As usual in QM, a symmetry is described by an operator $\mathcal{H} \to \mathcal{H}$ leaving the Hamiltonian is invariant. In our case the nontrivial part concerns the matching condition: a particular symmetry is associated with an invertible map in the space of the boundary values, $\Theta : \mathbb{C}^n \to \mathbb{C}^n$, such that we have $(U-I)\Theta\Psi(0) + i(U+I)\Theta\Psi'(0) = 0$ for all admissible Ψ, or equivalently

$$\Theta^{-1} U \Theta = U.$$

One asks which operators are associated with the parity and time reversal transformations. The latter is simpler. Operator $\Theta_{\mathcal{T}}$ is *antilinear* and *idempotent*, in the absence of internal degrees of freedom it is just the *complex conjugation*. Using the unitarity, $U^T \bar{U} = \bar{U} U^T = I$ we see that $\bar{\Psi}$ satisfies the matching condition with the *transposed matrix*, that is,

$$\Theta_{\mathcal{T}}^{-1} U \Theta_{\mathcal{T}} = \Theta_{\mathcal{T}} U \Theta_{\mathcal{T}} = U^T,$$

and consequently, the *H_U is $\mathcal{T}$-invariant if and only if $U = U^T$*.

How to describe mirror transformations?

This also immediately implies that a (self-adjoint) quantum graph *is $\mathcal{PT}$-symmetric if and only if the mirror transformation acts analogously,*

$$\Theta_{\mathcal{P}}^{-1} U \Theta_{\mathcal{P}} = \Theta_{\mathcal{P}} U \Theta_{\mathcal{P}} = U^T .$$

Note that the QG concept *per se* does not need an ambient space, but investigation of spatial reflections forces us to think of embedding in the Euclidean space. For simplicity we regard our star graph as *planar*, but the conclusion certainly extends to more general situations.

Note that $\Theta_{\mathcal{P}}$ does not mean to reverse the edge orientation as they are all parametrized in the same outward direction. Neither is $\Theta_{\mathcal{P}}$ associated with reversing the edge numeration; that leads to a double transpose of U, both with respect to the diagonal and antidiagonal, however, such a change means just renaming the graph edges.

To see which operator can facilitate the similarity between U and U^T, we use the *unitarity* of the matrix: there is a unitary V such that VUV^* is *diagonal*, and as such equal to its transpose. It follows that the matrix Θ satisfying $\Theta U \Theta = U^T$ is of the form $\Theta = V^T V$.

How to describe mirror transformations?

We know how V looks like: the jth column of V^* coincides with ϕ_j^T, where ϕ_j is the jth normalized eigenvector of U. Consequently, we have

$$\Theta_{ij} = (\bar{\phi}_i, \phi_j), \quad i, j = 1, \dots, n\,;$$

the expression is nontrivial due to complex conjugation in the left entry.

Denoting by $\{\nu_j\}$ the 'natural' basis in the boundary value space, namely $\nu_1 = (1, 0, \dots, 0)^T$, etc., we see that the above operator Θ maps ν_j to $((\bar{\phi}_1, \phi_j), \dots (\bar{\phi}_n, \phi_j))^T$, so it general it is difficult to associate such a Θ with a mirror transformation.

The situation changes, however, when we restrict our attention to the subset of *circulant* matrices, i.e. those of the form

$$U = \begin{pmatrix} c_1 & c_2 & \cdots & c_{n-1} & c_n \\ c_n & c_1 & c_2 & & c_{n-1} \\ \vdots & c_n & c_1 & \ddots & \vdots \\ c_3 & & \ddots & \ddots & c_2 \\ c_2 & c_3 & \cdots & c_n & c_1 \end{pmatrix}.$$

Circulant matrices

The unitarity requires that

$$c_j = \frac{1}{n}\left(\lambda_1 + \lambda_2\omega^{-j} + \lambda_3\omega^{-2j} + \cdots + \lambda_n\omega^{-(n-1)j}\right), \quad j = 1, \ldots, n,$$

where λ_j, $j = 1, \ldots, n$, are eigenvalues of U and $\omega := \mathrm{e}^{2\pi i/n}$. The corresponding eigenvectors are independent of the choice of the c_j's,

$$\phi_j = \frac{1}{\sqrt{n}}\left(1, \omega^j, \omega^{2j}, \ldots, \omega^{(n-1)j}\right)^T, \quad j = 1, \ldots, n.$$

Furthermore, the eigenvalues can be written in terms of the matrix entries as $\lambda_j = \sum_{k=1}^n c_k \omega^{j(k-1)}$. The diagonalization is achieved in this case by the *discrete Fourier transformation*,

$$V^* = \frac{1}{\sqrt{n}}\begin{pmatrix} 1 & 1 & 1 & 1 & \ldots & 1 \\ 1 & \omega & \omega^2 & \omega^3 & \ldots & \omega^{(n-1)} \\ 1 & \omega^2 & \omega^4 & \omega^6 & \ldots & \omega^{2(n-1)} \\ \vdots & \vdots & \vdots & \vdots & & \vdots \\ 1 & \omega^{n-1} & \omega^{2(n-1)} & \omega^{3(n-1)} & \ldots & \omega^{(n-1)^2} \end{pmatrix}.$$

Mirror transformation for circulant matrices

$$\Theta_{\mathcal{P}} = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 & 1 \\ 0 & 0 & 0 & \cdots & 0 & 1 & 0 \\ \vdots & & & \iddots & & & \vdots \\ 0 & 0 & 1 & \cdots & 0 & 0 & 0 \\ 0 & 1 & 0 & \cdots & 0 & 0 & 0 \end{pmatrix}$$

This has the needed properties, preserving the edge e_1, as well as e_{k+1} if $n = 2k$, and among the remaining ones *it switches e_j with e_{n+2-j}*, and moreover, the same will be true if we renumber the edges.

Thus we have found a class of vertex couplings *exhibiting a $\mathcal{PT}$-symmetry*. It depends on n real parameters, out of the number n^2 which characterize an arbitrary self-adjoint coupling. Among them, a subset depending on $[\frac{n}{2}] + 1$ parameters is *separately symmetric* with respect to the time inversion and mirror transformation, while in the $[\frac{n-1}{2}]$-parameter complement *the $\mathcal{PT}$-symmetry is nontrivial*.

The examples we discussed above belong, of course, to the latter subset.

A purely Robin coupling

To elucidate further the role played by the *absence of the Dirichlet component* in the vertex coupling, consider another interpolation: the coupling with

$$U = \epsilon R, \quad \epsilon = \mathrm{e}^{i\mu}, \quad \mu \in \left(0, \tfrac{2\pi}{n}\right)$$

having the eigenvalue -1 at the endpoints of the parameter interval only.

In components the matching condition in this case reads

$$\epsilon\psi_{j+1} - \psi_j + i\ell(\epsilon\psi'_{j+1} + \psi'_j) = 0 \pmod n$$

and its $\mathcal{PT}$-symmetry is obvious. Putting $\eta := \frac{1-k\ell}{1+k\ell}$ we find

$$S_{ij}(k) = \frac{1}{1-\epsilon^n\eta^n}\Big(-\eta(1-\epsilon^n\eta^{n-2})\delta_{ij} + (1-\delta_{ij})(1-\eta^2)\epsilon(\epsilon\eta)^{(j-i-1)(\mathrm{mod}\, n)}\Big).$$

We have now $\lim_{k\to\infty} S(k) = I$ because of the factor $1-\eta^2$ which cancels out with the prefactor only if $\epsilon = 1$.

To see how the spectrum changes, let us revisit the square lattice example.

P.E., M. Tater: Quantum graphs: self-adjoint, and yet exhibiting a nontrivial $\mathcal{PT}$-symmetry, *Phys. Lett.* **A416** (2021), 127669

Square lattice example revisited

In the elementary cell of the lattice, we use again the Ansatz

$$\psi_1(x) = a_1 \mathrm{e}^{ikx} + b_1 \mathrm{e}^{-ikx}, \psi_2(x) = a_2 \mathrm{e}^{ikx} + b_2 \mathrm{e}^{-ikx},$$

$$\psi_3(x) = \omega_1 \left(a_1 \mathrm{e}^{ik(x+\ell)} + b_1 \mathrm{e}^{-ik(x+\ell)} \right), \psi_4(x) = \omega_2 \left(a_2 \mathrm{e}^{ik(x+\ell)} + b_2 \mathrm{e}^{-ik(x+\ell)} \right).$$

Using the mentioned matching condition and Floquet at the 'loose' ends, we get a linear system which is solvable if the determinant

$$D \equiv D(\eta, \omega_1, \omega_2) = \begin{vmatrix} -1 & -\eta & \epsilon\eta & \epsilon \\ \epsilon\omega_1\xi^2 & \epsilon\omega_1\bar{\xi}^2\eta & -1 & -\eta \\ -\omega_1\xi^2\eta & -\omega_1\bar{\xi}^2 & \epsilon\omega_2\xi^2 & \epsilon\omega_2\bar{\xi}^2\eta \\ \epsilon\eta & \epsilon & -\omega_2\xi^2\eta & -\omega_2\bar{\xi}^2 \end{vmatrix},$$

where $\omega_j = \mathrm{e}^{i\theta_j}$, $\xi = \mathrm{e}^{ik\ell}$ and $\epsilon = \mathrm{e}^{i\mu}$ with $\mu \in \left(0, \frac{1}{2}\pi\right)$ vanishes. This gives

$$8i\epsilon^2 \frac{\mathrm{e}^{i(\theta_1+\theta_2)}}{(k+1)^4} \sum_{j=0}^{4} c_j k^j = 0,$$

where

$$c_0 = c_4 = -\sin 2\mu \, \sin^2 k\ell, \quad c_2 = \sin 2\mu \, (1 + 3\cos 2k\ell),$$

$$c_1 = 2\big(2\cos 2\mu \, \cos k\ell - \cos\theta_1 - \cos\theta_2\big) \sin k\ell,$$

$$c_3 = 2\big(2\cos 2\mu \, \cos k\ell + \cos\theta_1 + \cos\theta_2\big) \sin k\ell;$$

for the negative spectrum one has to set $k = i\kappa$ with $\kappa > 0$.

Spectral properties

If $\mu = 0$ the even c_j's are zero and we get the solution discussed above, in particular, the positive spectrum is *dominated by bands* growing linearly.

This changes once we have $\mu \neq 0$. The form of c_2 does not allow to factorize a θ-independent term so *there is no infinite series of flat bands*. This does not mean that the point spectrum is void, though. Choosing $k = 1$, the spectral condition reduces to $\sum_{j=0}^{4} c_j = 0$ where the θ-dependent terms cancel and the sum vanishes provided

$$\cot 2\mu = \frac{-1 - 3\cos 2\ell + 2\sin^2 \ell}{4 \sin 2\ell} = -\cot 2\ell,$$

that is, we have a *flat band* at $\mu = \frac{\pi}{2} - \ell \pmod{\frac{\pi}{2}}$.

We lack now the nice graphical solution we had for $\mu = 0$, but it is not difficult to determine the high-energy asymptotic behavior. Since $c_4 \neq 0$ for $k \neq \frac{\pi n}{\ell}$, spectral bands may exist only *in the vicinity of* $\left(\frac{\pi n}{\ell}\right)^2$, while these point themselves do not belong to $\sigma(H_U)$.

Spectral properties, continued

Furthermore, the width of the nth band on the energy scale is *for a fixed $\mu \in \left(0, \frac{\pi}{2}\right)$ asymptotically constant*,

$$\Delta_n \lesssim \frac{8}{\ell} \cot \mu .$$

We stress the fixed value of μ. The band width is not monotonous over the whole interval $\left[0, \frac{\pi}{2}\right]$; as we are approaching the right endpoint, it starts growing again, because $U = iR$ too *has -1 as its eigenvalue*.

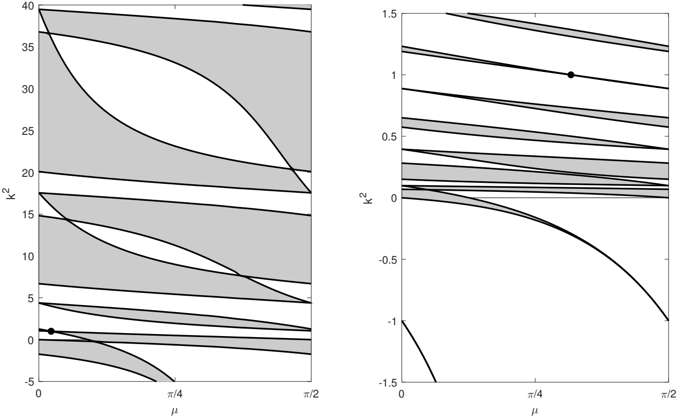
This non-uniform character is also manifested by the fact that we have

$$P_\sigma(H_U) := \lim_{K\to\infty} \frac{1}{K} \left|\sigma(H_U) \cap [0, K]\right| = 0, \quad \mu \in \left(0, \tfrac{\pi}{2}\right),$$

while for both the real-valued $U = R$ and the purely imaginary $U = iR$ the probability is equal to one.

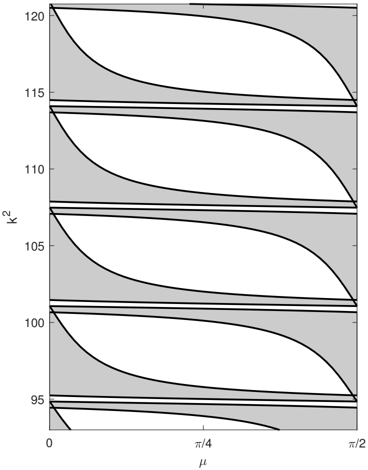
The negative spectrum of H_U has *two bands*. In particular, for large ℓ they are narrow and to shrink to the star-graph eigenvalues referring to $\kappa = \tan \frac{\mu}{2}$ and $\tan\left(\frac{\mu}{2} + \frac{\pi}{4}\right)$ as $\kappa \to \infty$.

The spectrum as a function of μ



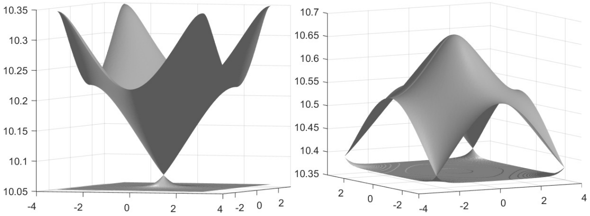
The spectrum of H_U for $\ell = \frac{3}{2}$ and $\ell = 10$, respectively. The dot indicates the flat band at $k = 1$.

High-energy spectrum



The spectrum for $\ell = 10$ again: for a fixed $\mu \in \left(0, \frac{\pi}{2}\right)$ the positive spectral bands get narrower as the energy grows, while at the endpoints of the interval they dominate the spectrum.

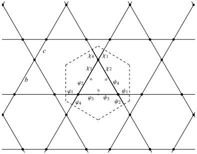
Closing gaps



In distinction to the flat band at $(\mu, k) = \left(\frac{\pi}{2} - \ell, 1\right)$ we have *true band crossings* occurring either in the center of the Brillouin zone or its corners. Here we have dispersion surfaces (in the momentum variable) for $\ell = 10$ at the points of closing gaps, left at $(\mu, k) = (1.55068665, 10.07328547)$, right at $(\mu, k) = (1.55190524, 10.38681556)$. The picture clearly shows the *Dirac cones* at the touching points.

Back to couplings with the Dirichlet component

One can analyze other examples such as *Kagome lattice* with the coupling $U = R$ and its degenerate case, the *triangular lattice*



One conclusion is the confirmation of *Band-Berkolaiko universality*: whenever the edges are *incommensurate*, we have

$$P_\sigma(H_U) := \lim_{K\to\infty} \frac{1}{K} |\sigma(H_U) \cap [0, K]| \approx 0.639.$$

M. Baradaran, P.E.: Kagome network with vertex coupling of a preferred orientation, arXiv:2106.16019

On the other hand, the Dirichlet component is present in some 'usual' couplings, in the first place the *δ-coupling*; lattices with this coupling have $P_\sigma(H_U) = 1$. This does not mean, however, that the spectrum cannot exhibit interesting features.

Let us ask how many spectral gaps are open

To motivate this question, recall first that for the 'usual' Schrödinger operators the dimension is known to be decisive: systems which are *$\mathbb{Z}$-periodic* have generically an *infinite number* of open gaps, while *$\mathbb{Z}^\nu$-periodic systems with $\nu \geq 2$* have only *finitely many* open gaps

This is the celebrated *Bethe–Sommerfeld conjecture*, rather plausible for the physicist's point of view but mathematically quite hard, to which we have nowadays an affirmative answer in a large number of cases

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?

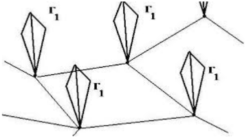
The standard reference, [Berkolaiko-Kuchment'13], says that Bethe-Sommerfeld heuristic reasoning is applicable again, however, the finiteness of the gap number *is not a strict law*

Graph decoration

An infinite number of gaps in the spectrum of a periodic graph can result from *decorating* its vertices by copies of a fixed compact graph. This fact was observed first in the *combinatorial graph context*,

J.H. Schenker, M. Aizenman: The creation of spectral gaps by graph decoration, *Lett. Math. Phys.* **53** (2000), 253–262.

and the argument extends easily to metric graphs we consider here



Courtesy: Peter Kuchment

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*

Most graphs are not Bethe-Sommerfeld

To begin with, Band-Berkolaiko universality suggests that examples – if they exist – must be sought among lattices satisfying $P_\sigma(H_U) = 1$ and it is also clear that the coupling must have a Dirichlet component.

This is not sufficient, though. Consider, for instance, couplings *without the Robin component*. We call them *scale-invariant* since the matching conditions $(U - I)\psi + i(U + I)\psi' = 0$, then splits and the transport through such a vertex is *energy independent*; a prime example of such a condition is the *Kirchhoff coupling*. We have

Theorem

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

P.E., O. Turek: Periodic quantum graphs from the Bethe-Sommerfeld perspective, *J. Phys. A: Math. Theor.* **50** (2017), 455201.

More generally, it is shown in this paper that if a scale invariant coupling at vertices of a periodic lattice has *at least one open gap*, then any coupling *with the same Dirichlet part* yields infinitely many gaps.

The existence

Nevertheless, the answer to our question is affirmative:

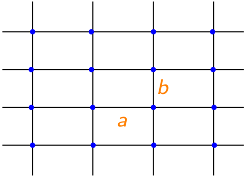
Theorem

Bethe–Sommerfeld graphs exist.

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

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

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

The spectrum depends on the ratio $\theta = \frac{a}{b}$. If θ is rational, $\sigma(H)$ has clearly 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 continued fraction representation $\theta = [a_0; a_1, a_2, \dots]$ 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 $q \neq 0$.

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*

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

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.

The proof [E-Turek, loc.cit.] is based on Diophantine approximations.

Corollary

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

More about this example

The window in which the golden-mean lattice has the BS property is *narrow*, it is roughly $4.298 \lesssim -\alpha a \lesssim 4.414$.

We are also able to control the number of gaps in the BS regime; in the same paper the following result was proved:

Theorem

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

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

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

$$A_j < \frac{\pi^2}{\sqrt{5}} \quad \text{holds for all } j \in \mathbb{N}\,.$$

A more general result

Theorem

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 $\lceil\cdot\rceil$ and $\tan$ by $-\tan$. If the coupling α satisfies

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

where $\mu(\theta) := \inf\left\{ c>0 \,\middle|\, (\exists_\infty (p,q)\in\mathbb{N}^2)\left(\left|\theta - \frac{p}{q}\right| < \frac{c}{q^2}\right)\right\}$ is the Markov constant, then there is a nonzero and finite number of gaps in the positive spectrum.

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.

In connection with the previous discussion, a *natural question* arises: is there a lattice with the coupling which $\mathcal{PT}$-symmetric but *not* $\mathcal{T}$-symmetric which would have the Bethe-Sommerfeld property?

And finally, where is the ergodicity?

In finite graphs with *even degree vertices* one can observe a *quantum chaos* which is, interestingly, of *GOE type* even if the time-reversal invariance is violated – a *work in progress* with Rami and his students.

It could also be interesting to make the parameters in infinite periodic graphs *random i.i.d. variables* asking about *(de)localization*, for instance

- Lattices with the $(\psi_{j+1} - \psi_j) + i\ell(\psi'_{j+1} + \psi'_j) = 0$ coupling with a random ℓ, comparing the square and hexagonal case
- A loose ring chain with the link length ℓ, comparing the regimes where the latter is chosen randomly in $(0, \ell_0)$ and *away from zero*
- A square lattice with the coupling $U = \mathrm{e}^{i\mu} R$, comparing the regimes when $\mu \in (-\mu_0, \mu_0)$ and *away from multiples of* $\frac{\pi}{2}$
- etc.

Instead of randomness, one can consider situations where the lengths and/or coupling parameters are *quasiperiodic*, etc.

It remains to say

Thank you for your attention!