Effects of time-reversal asymmetry in the vertex coupling of quantum graphs

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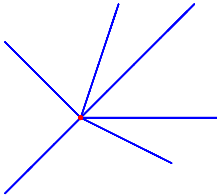
Recall that to define a QM Hamiltonian, in general it is not sufficient to specify its differential symbol. To qualify as an observable, the operator must be *self-adjoint*, $H = H^*$, which for an unbounded operator is a considerably stronger requirement than mere *symmetry*, $H \subset H^*$.

In physicist's language this means to demand that that the *probability current must be preserved*. Let us illustrate that on an example:



The most simple case is a *star graph* with the state Hilbert space $\mathcal{H} = \bigoplus_{j=1}^{n} L^2(\mathbb{R}_+)$ and the particle Hamiltonian acting on $\mathcal{H}$ as $\psi_j \mapsto -\psi_j''$

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These boundary values can be written as columns, $\Psi(0) := \{\psi_j(0)\}$ and $\Psi'(0) := \{\psi'_j(0)\}$, the entries 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

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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*.

Vertex coupling

The claim is easy to verify. To see that it is enough to express the squared norms $\|\Psi(0) \pm i\ell\Psi'(0)\|^2_{\mathbb{C}^n}$ and subtract them from each other; the difference is nothing but the *boundary form*,

$$(H\psi, \psi) - (\psi, H\psi) = \sum_{j=1}^{n} (\bar{\psi}_j \psi'_j - \bar{\psi}'_j \psi_j)(0) = 0,$$

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It seems that we have one more parameter, but it is not important because the matrices corresponding to two different values are related by

$$U' = \frac{(\ell + \ell')U + \ell - \ell'}{(\ell - \ell')U + \ell + \ell'}.$$

Thus we can set $\ell = 1$, which means just a *choice of the length scale*.

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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.

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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*.

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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*,

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

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- Similarly, $U = I - \frac{2}{n-i\beta}\mathcal{J}$ describes the *δ_{s}' coupling*,
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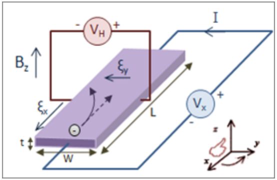
with $U = \frac{n-i\alpha}{n+i\alpha} I - \frac{2}{n+i\alpha}\mathcal{J}$ and Neumann edge decoupling for $\beta = \infty$.
- But there are many other couplings, and one can choose *ad hoc* to fit the physics of the problem.

Hall effect

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



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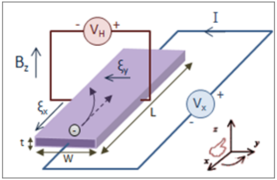

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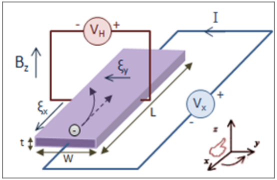

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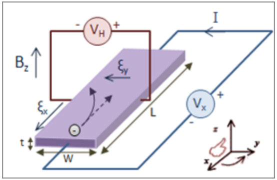

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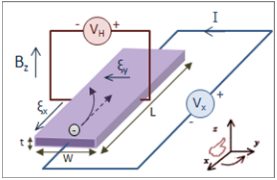

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In contrast to the 'usual' quantum Hall effect, its mechanism is not well understood; it is conjectured that it comes from *internal magnetization* in combination with the *spin-orbit interaction*.

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 have seen already)

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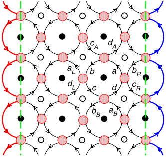

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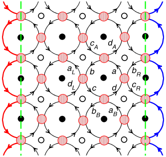

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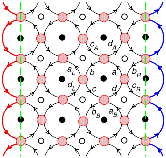

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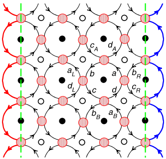

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Looking at the picture we recognize a *flaw in the model*: to mimick the rotational motion of atomic orbitals responsible for the magnetization, the authors had to impose 'by hand' the requirement that the electrons move only one way on the loops of the lattice. Naturally, such an assumption *cannot be justified from the first principles!*

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

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

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

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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.*

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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

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

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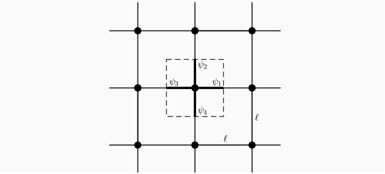
Let us look how this fact influences spectra of *periodic* quantum graphs.

Comparison of two lattices



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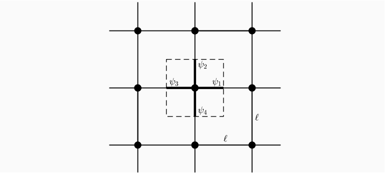

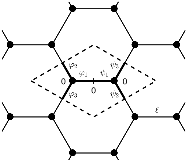

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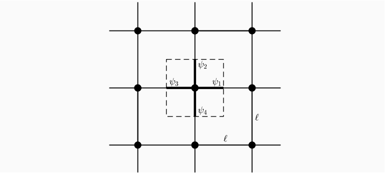

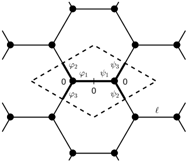

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$$16i\,\mathrm{e}^{i(\theta_1+\theta_2)}\,k\,\sin k\ell\big[(k^2-1)(\cos\theta_1+\cos\theta_2)+2(k^2+1)\cos k\ell\big]=0$$

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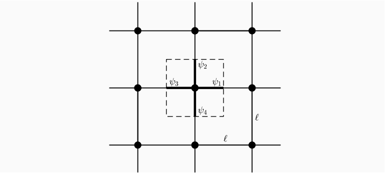

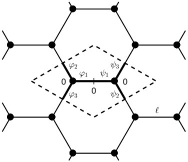

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where $d_\theta := \cos\theta_1+\cos(\theta_1-\theta_2)+\cos\theta_2$ and $\frac{1}{\ell}(\theta_1,\theta_2)\in[-\frac{\pi}{\ell},\frac{\pi}{\ell}]^2$ is the quasimomentum

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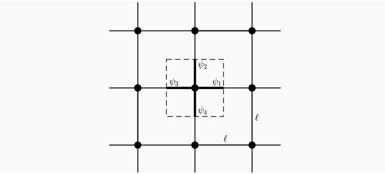

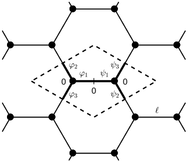

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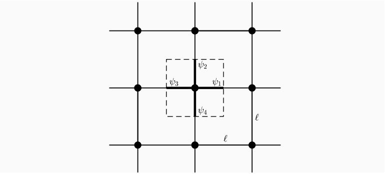

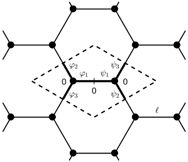

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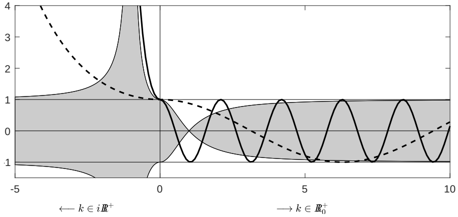
P.E., M. Tater: Quantum graphs with vertices of a preferred orientation, *Phys. Lett.* **A382** (2018), 283–287.

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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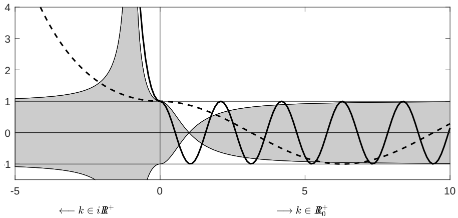

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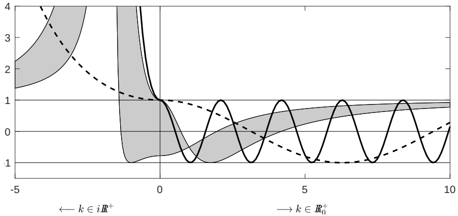

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Let us mention one more involved choice of the vertex coupling.

An interpolation

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

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

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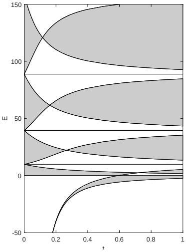

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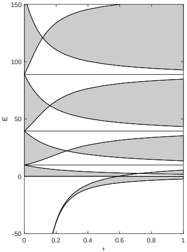

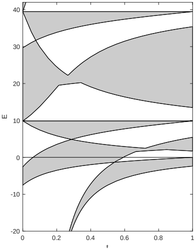

P.E., O. Turek, M. Tater: A family of quantum graph vertex couplings interpolating between different symmetries, *J. Phys. A: Math. Theor.* **51** (2018), 285301.

Another topic: band edges positions

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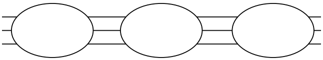

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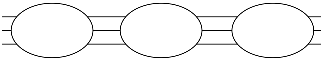

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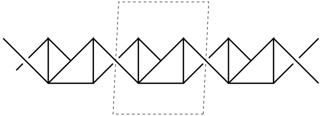

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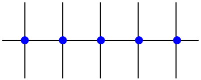

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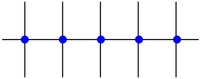

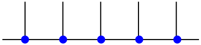

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Band edges, continued

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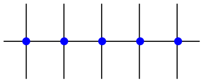

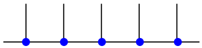

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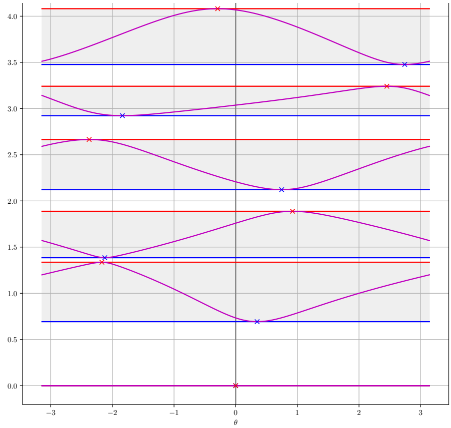
Two-sided comb: dispersion curves



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

Discrete symmetry: Platonic solid graphs

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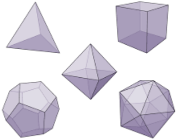

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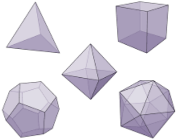

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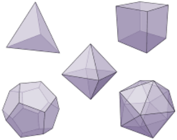

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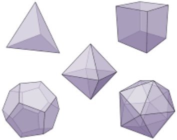

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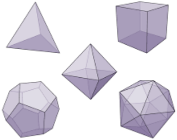

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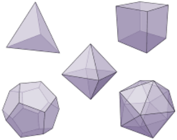

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P.E., J. Lipovský: Spectral asymptotics of the Laplacian on Platonic solids graphs, *J. Math. Phys.* **60** (2019), 122101

Another periodic graph model

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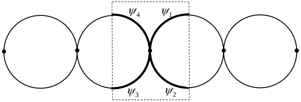
Let us look what this coupling influences graphs *periodic in one direction*. Consider again a *loop chain*, first *tightly connected*



The spectrum of the corresponding Hamiltonian looks as follows:

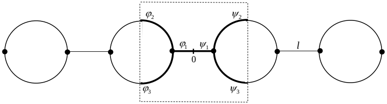
Theorem

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.



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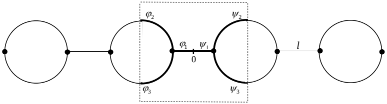

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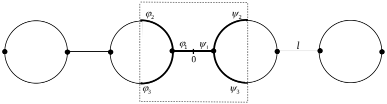

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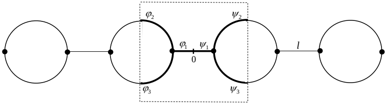

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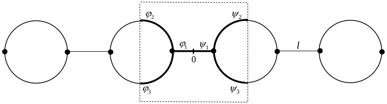

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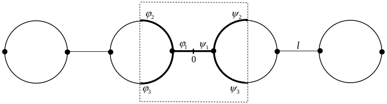

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- *The positive spectrum has infinitely many gaps.*
- $P_\sigma(H_\ell) := \lim_{K\to\infty} \frac{1}{K} |\sigma(H_\ell) \cap [0, K]| = 0$ *holds for any $\ell > 0$.*

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*, which was introduced in

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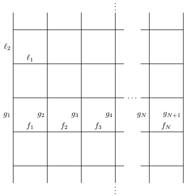
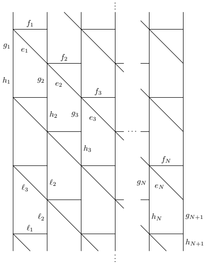
Note also that if we violate the mirror symmetry of the chain, we have instead $P_\sigma(H_0) = \frac{1}{2}$ independently of where exactly we place the vertex.

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:





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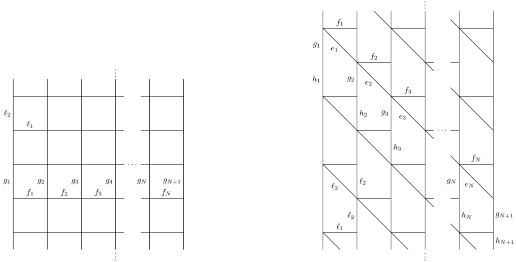

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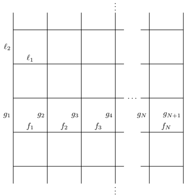

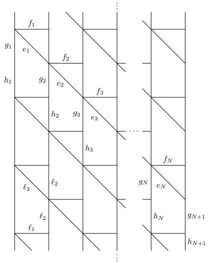

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This time we ask in which part of the 'guide' are the generalized eigenfunction *dominantly supported*

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!

$\mathcal{PT}$-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.

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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

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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

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

Vertex coupling symmetries

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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,*

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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

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

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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.

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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

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

where λ_j, $j = 1, \dots, n$, 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,

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

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*,

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

Mirror transformation for circulant matrices

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

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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.

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

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

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Thank you for your attention!