



Guided quantum dynamics

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With thanks to all my collaborators

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on Mathematics for the Micro/Nano-World

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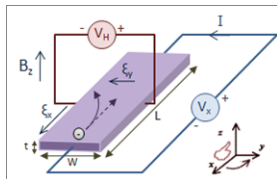
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- Concerning the terminology: at the beginning one spoke about *QM on graphs*. The term *quantum graph* was coined by Uzy Smilansky at the end of the 90s, and he later expressed regrets about that.

Hall effect



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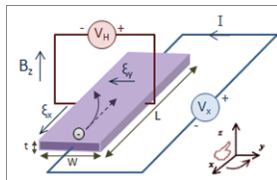
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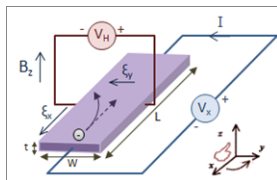
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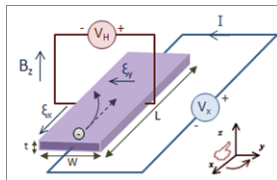
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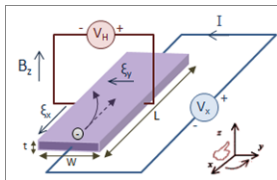
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In contrast to the 'usual' quantum Hall effect, its mechanism is not well understood; it is conjectured that it comes from *internal magnetization* in combination with the *spin-orbit interaction*.

Modeling anomalous Hall effect



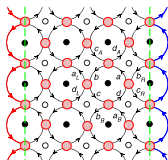
Recently a *quantum-graph model* of the AHE was proposed in which the material structure of the sample is described by lattice of δ -coupled rings (topologically equivalent to the *square lattice* we will discuss later)



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



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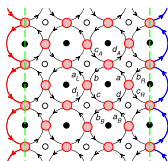
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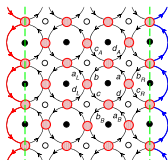
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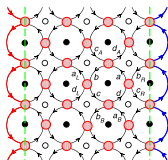
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Looking at the picture we recognize a *flaw in the model*: to mimick the rotational motion of atomic orbitals responsible for the magnetization, the authors had to impose 'by hand' the requirement that the electrons move only one way on the loops of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

Breaking the time-reversal invariance



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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

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

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

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Star graphs: spectrum and scattering



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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

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

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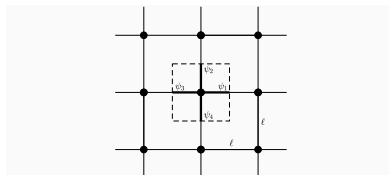
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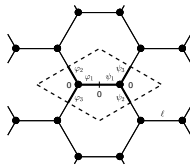
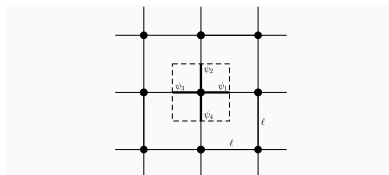
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Let us look how this fact influences spectra of *periodic* quantum graphs.

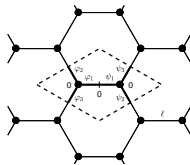
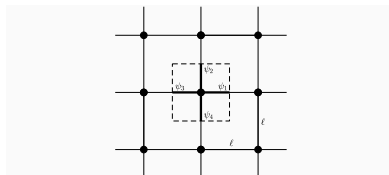
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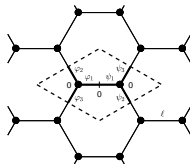
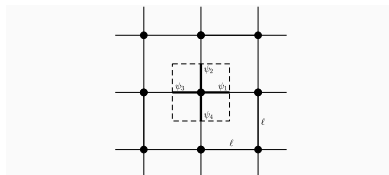
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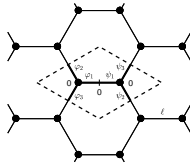
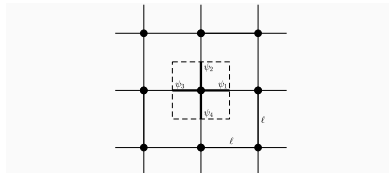
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where $d_\theta := \cos \theta_1 + \cos(\theta_1 - \theta_2) + \cos \theta_2$ and $\frac{1}{\ell}(\theta_1, \theta_2) \in [-\frac{\pi}{\ell}, \frac{\pi}{\ell}]^2$ is the quasimomentum

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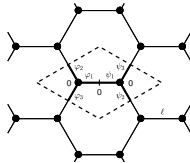
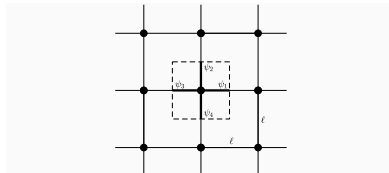
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where $d_\theta := \cos \theta_1 + \cos(\theta_1 - \theta_2) + \cos \theta_2$ and $\frac{1}{\ell}(\theta_1, \theta_2) \in [-\frac{\pi}{\ell}, \frac{\pi}{\ell}]^2$ is the quasimomentum. They are tedious to solve except the *flat band cases*, $\sin k\ell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

Comparison of two lattices



Spectral condition for the two cases are easy to derive,

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

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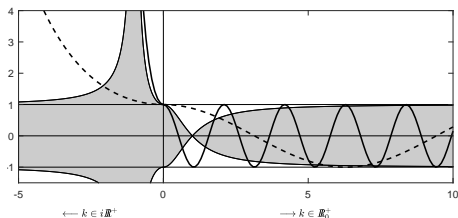


P.E., M. Tater: Quantum graphs with vertices of a preferred orientation, *Phys. Lett.* **A382** (2018), 283–287.

A picture is worth of thousand words



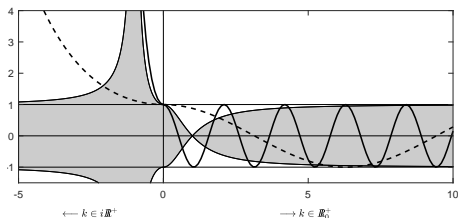
For the two lattices, respectively, we get (with $\ell = \frac{3}{2}$, dashed $\ell = \frac{1}{4}$)



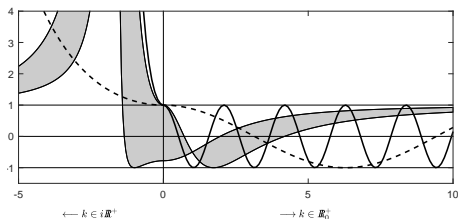
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Comparison summary



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- the number of open gaps is *always infinite*

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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

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

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

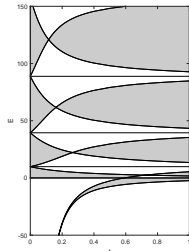
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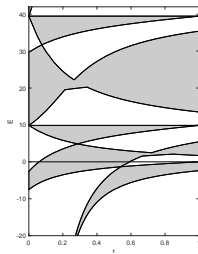
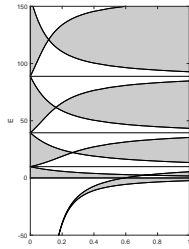
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P.E., O. Turek, M. Tater: A family of quantum graph vertex couplings interpolating between different symmetries, *J. Phys. A: Math. Theor.* **51** (2018), 285301.

Another topic: band edges positions

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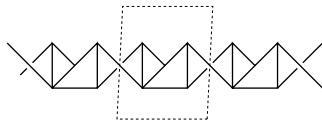


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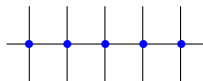
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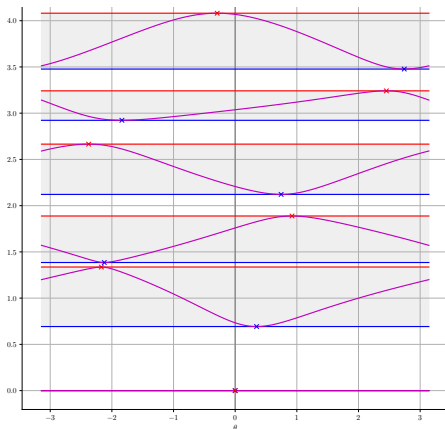
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- and what about the dispersion curves?

Two-sided comb: dispersion curves



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

Discrete symmetry: Platonic solid graphs

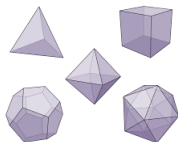
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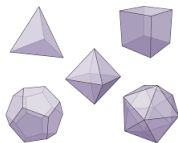
Source: Wikipedia Commons

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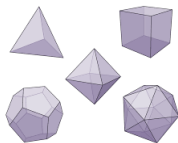
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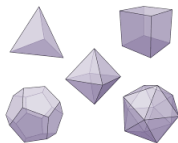
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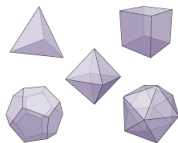
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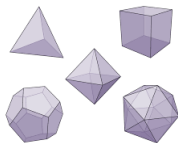
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P.E., J. Lipovský: Spectral asymptotics of the Laplacian on Platonic solids graphs, *J. Math. Phys.* **60** (2019), 122101

Another periodic graph model

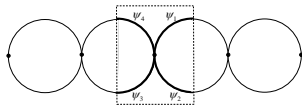


Let us look what this coupling influences graphs *periodic in one direction*

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.

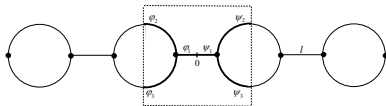


M. Baradaran, P.E., M. Tater: Ring chains with vertex coupling of a preferred orientation, *Rev. Math. Phys.* **33** (2021), 2060005.

A loosely connected chain



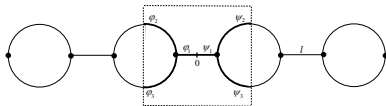
Replace the direct coupling of adjacent rings by connecting segments of length $\ell > 0$, still with the same vertex coupling.



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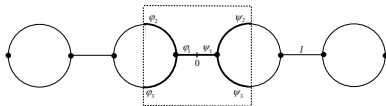
The spectrum of H_ℓ has for any fixed $\ell > 0$ the following properties:

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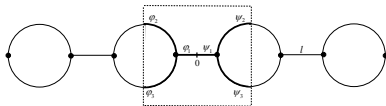
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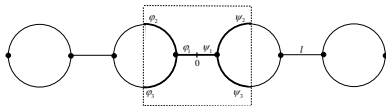
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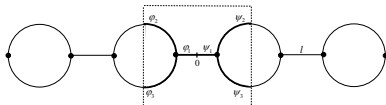
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- $P_\sigma(H_\ell) := \lim_{K \rightarrow \infty} \frac{1}{K} |\sigma(H_\ell) \cap [0, K]| = 0$ holds for any $\ell > 0$.

The limit $\ell \rightarrow 0+$



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.

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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!*

The limit $\ell \rightarrow 0+$



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 $\sigma(H_\ell) \rightarrow \sigma(H_0)$ *in the set sense* as $\ell \rightarrow 0+$.

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 (irrationality not needed due the very simple form of spectral condition).

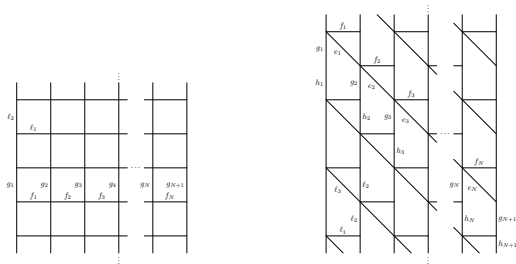


M. Baradaran, P.E., M. Tater: Spectrum of periodic chain graphs with time-reversal non-invariant vertex coupling, *Ann. Phys.* **443** (2022), 168992

One more example: transport properties



Consider strips cut of the following two types of lattices:

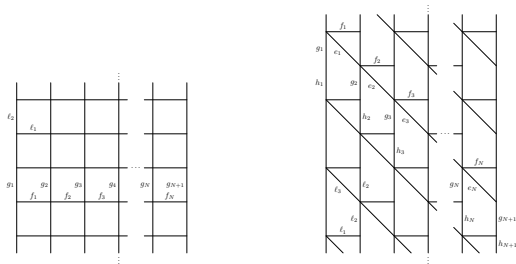


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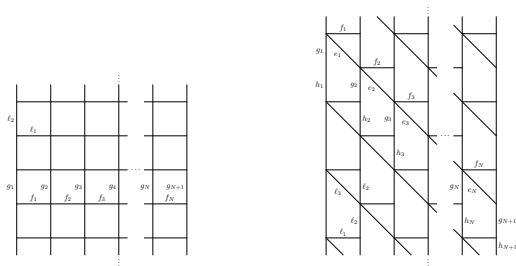


In both cases we impose the ‘rotating’ coupling at the vertices. By Floquet decomposition we are able reduce the task to investigation of a ‘one cell layer’. We use the Ansatz $ae^{ikx} + be^{-ikx}$ for the wave functions e, f_j, g_j, h_j with the appropriate coefficients at the graphs edges

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

Theorem

- *In the rectangular-lattice strip, for a fixed $K \in (0, \frac{1}{2}\pi)$, 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 $k \rightarrow \infty$.*

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

$$k \notin \bigcup_{n \in \mathbb{N}_0} \left(\frac{n\pi - K}{l_1}, \frac{n\pi + K}{l_1} \right) \cup \bigcup_{n \in \mathbb{N}_0} \left(\frac{n\pi - K}{l_2}, \frac{n\pi + K}{l_2} \right) \cup \bigcup_{n \in \mathbb{N}_0} \left(\frac{n\pi - K}{l_3}, \frac{n\pi + K}{l_3} \right).$$

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 $k \rightarrow \infty$.



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. Krejčířík, 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.



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As usual in QM, a symmetry is described by an operator $\mathcal{H} \rightarrow \mathcal{H}$ leaving the Hamiltonian 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, $\Theta : \mathbb{C}^n \rightarrow \mathbb{C}^n$, such that we have $(U - I)\Theta\Psi(0) + i(U + I)\Theta\Psi'(0) = 0$ for all admissible Ψ , or equivalently

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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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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.

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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 j th column of V^* coincides with ϕ_j^T , where ϕ_j is the j th 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 in 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

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

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

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

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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*,

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

Mirror transformation for circulant matrices



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

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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 n real parameters, out of the number n^2 which characterize an arbitrary self-adjoint coupling. Among them, a subset depending on $\lfloor \frac{n}{2} \rfloor + 1$ parameters is *separately symmetric* with respect to the time inversion and mirror transformation, while in the $\lfloor \frac{n-1}{2} \rfloor$ -parameter complement *the \mathcal{PT} -symmetry is nontrivial*.

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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

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

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

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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

$$S_{ij}(k) = \frac{1}{1 - \epsilon^n \eta^n} \left(-\eta(1 - \epsilon^n \eta^{n-2})\delta_{ij} + (1 - \delta_{ij})(1 - \eta^2)\epsilon(\epsilon\eta)^{(j-i-1) \pmod{n}} \right).$$

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

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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

$$\begin{aligned}\psi_1(x) &= a_1 e^{ikx} + b_1 e^{-ikx}, \psi_2(x) = a_2 e^{ikx} + b_2 e^{-ikx}, \\ \psi_3(x) &= \omega_1 \left(a_1 e^{ik(x+\ell)} + b_1 e^{-ik(x+\ell)} \right), \psi_4(x) = \omega_2 \left(a_2 e^{ik(x+\ell)} + b_2 e^{-ik(x+\ell)} \right).\end{aligned}$$

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 $\omega_j = e^{i\theta_j}$, $\xi = e^{ik\ell}$ and $\epsilon = e^{i\mu}$ with $\mu \in (0, \frac{1}{2}\pi)$ vanishes

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

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

where

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

$$c_1 = 2(2 \cos 2\mu \cos kl - \cos \theta_1 - \cos \theta_2) \sin kl,$$

$$c_3 = 2(2 \cos 2\mu \cos kl + \cos \theta_1 + \cos \theta_2) \sin kl;$$

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.

Spectral properties



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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* $(\frac{\pi n}{\ell})^2$, while these point themselves do not belong to $\sigma(H_U)$.

Spectral properties, continued



Furthermore, the width of the n th band on the energy scale is *for a fixed* $\mu \in (0, \frac{\pi}{2})$ *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 $[0, \frac{\pi}{2}]$; as we are approaching the right endpoint, it starts growing again, because $U = iR$ too *has -1 as its eigenvalue*.

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

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

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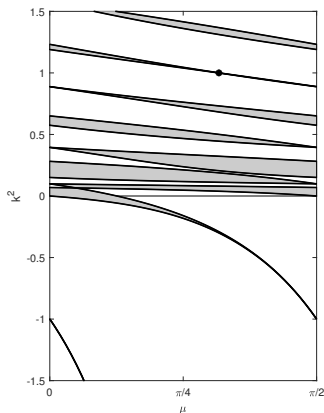
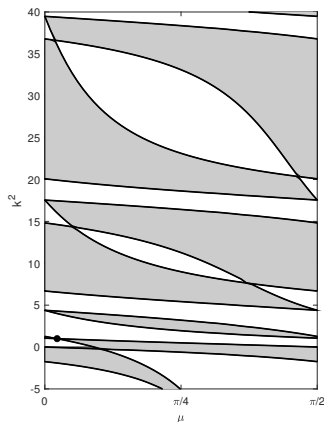
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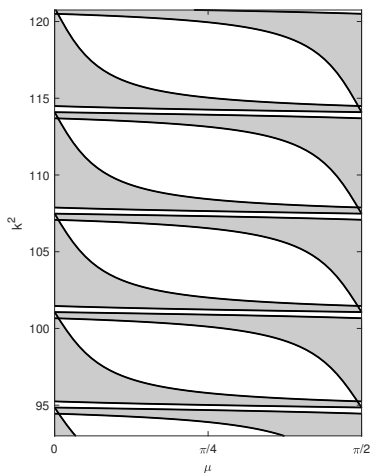
The negative spectrum of H_U has *two bands*. In particular, for large ℓ they are narrow and to shrink to the star-graph eigenvalues referring to $\kappa = \tan \frac{\mu}{2}$ and $\tan (\frac{\mu}{2} + \frac{\pi}{4})$ as $\kappa \rightarrow \infty$.

The spectrum as a function of μ



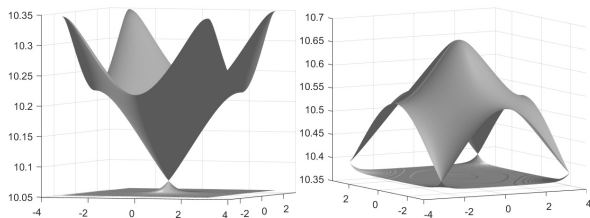
The spectrum of H_U for $\ell = \frac{3}{2}$ and $\ell = 10$, respectively. The dot indicates the flat band at $k = 1$.

High-energy spectrum



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

Closing gaps

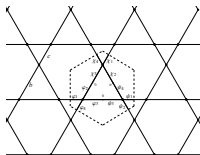


In distinction to the flat band at $(\mu, k) = (\frac{\pi}{2} - \ell, 1)$ we have *true band crossings* occurring either in the center of the Brillouin zone or its corners. Here we have dispersion surfaces (in the momentum variable) for $\ell = 10$ at the points of closing gaps, left at $(\mu, k) = (1.55068665,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

Returning to the original vertex coupling



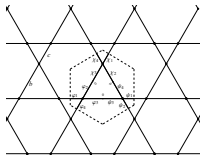
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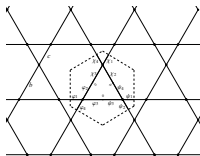


M. Baradaran, P.E.: Kagome network with vertex coupling of a preferred orientation, *J. Math. Phys.* **63** (2022), 083502

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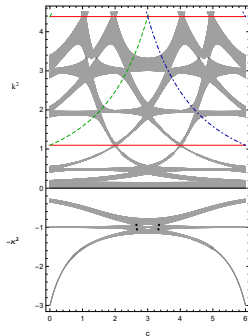
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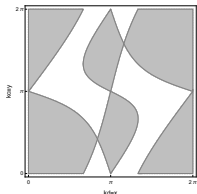
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To understand the reason, let us see how the spectral condition looks like,

$$0 \leq \frac{5}{4} + \frac{\cos kd \cos \frac{k(2c-d)}{2} + \cos \frac{3kd}{2}}{\cos \frac{k(2c-d)}{2} + \cos \frac{kd}{2}} \leq \frac{9}{4},$$

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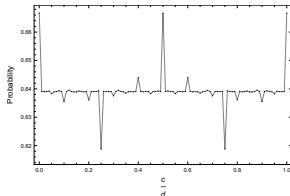
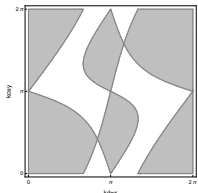
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To give one more example, let us mention the *Payne-Pólya-Weinberger inequality*: in the same situation the *ratio* of the first two eigenvalues, $\frac{\lambda_2(\Omega)}{\lambda_1(\Omega)}$, is sharply *maximized* by a ball.



M.S. Ashbaugh, R.D. Benguria: A sharp bound for the ratio of the first two eigenvalues of Dirichlet Laplacians and extensions, *Ann. Math.* **135** (1992), 601–628.

Non-simply connected regions

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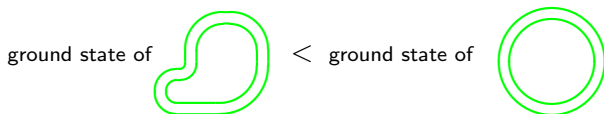


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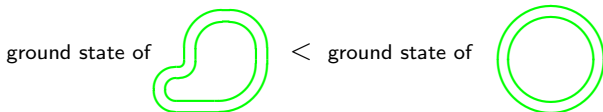


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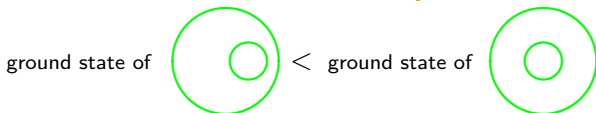


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Similarly, for a *circular obstacle in circular cavity* we have



whenever the obstacle is off center; the minimum is reached when it is touching the boundary.



E.M. Harrell, P. Kröger, K. Kurata: On the placement of an obstacle or a well so as to optimize the fundamental eigenvalue, *SIAM J. Math. Anal.* **33** (2001), 240–259.

A leaky loop analogue

Let Γ be a *loop* in \mathbb{R}^d , $d \geq 2$, parametrized by its arc length, i.e. a *piecewise differentiable* function $\Gamma : [0, L] \rightarrow \mathbb{R}^d$ such that $\Gamma(0) = \Gamma(L)$ and $|\dot{\Gamma}(s)| = 1$ for all but finitely many $s \in [0, L]$



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One more time, we employ the generalized *Birman-Schwinger principle* by which there is one-to-one correspondence between eigenvalues $-\kappa^2$ of $H_{\alpha, \Gamma}$ and solutions to the integral-operator equation

$$\mathcal{R}_{\alpha, \Gamma}^{\kappa} \phi = \phi, \quad \text{where } \mathcal{R}_{\alpha, \Gamma}^{\kappa}(s, s') := \frac{\alpha}{2\pi} K_0(\kappa |\Gamma(s) - \Gamma(s')|)$$

on $L^2([0, L])$, where K_0 is the Macdonald function.

Rephrasing it as a geometric problem



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Remark: The (reverse) inequalities hold also for $p \in [-2, 0)$ showing, e.g., that a *charged loop in the absence of gravity takes a circular form*.

A discrete analogue: polymer loops



Consider the same loop as above with *point interactions* placed at the *arc distances* $\frac{jL}{N}$, $j = 0, \dots, N_1$, in other words, the formal Hamiltonian

$$H_{\alpha, \Gamma}^N = -\Delta + \tilde{\alpha} \sum_{j=0}^{N-1} \delta\left(x - \Gamma\left(\frac{jL}{N}\right)\right)$$

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Introduce the *generalized boundary values* as the coefficients in the expansion of H_Y^* where H_Y is the Laplacian restricted to functions vanishing at the vicinity of the points of Y .

Point interactions ‘necklaces’



A reminder: fixing the points $y_j \in Y$ the said expansions look as

$$\psi(x) = -\frac{1}{2\pi} \log|x - y_j| L_0(\psi, y_j) + L_1(\psi, y_j) + \mathcal{O}(|x - y_j|), \quad d = 2,$$

$$\psi(x) = \frac{1}{4\pi|x - y_j|} L_0(\psi, y_j) + L_1(\psi, y_j) + \mathcal{O}(|x - y_j|), \quad d = 3.$$

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Theorem

The *ground state* of $H_{\alpha, \Gamma}^N$ is uniquely maximized by a *N-regular polygon*.



P.E.: Necklaces with interacting beads: isoperimetric problems, in Proceedings of the “International Conference on Differential Equations and Mathematical Physics” (Birmingham 2006), AMS *Contemporary Mathematics Series*, vol. 412, Providence, R.I., 2006; pp. 141-149.

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A reminder: fixing the points $y_j \in Y$ the said expansions look as

$$\psi(x) = -\frac{1}{2\pi} \log|x - y_j| L_0(\psi, y_j) + L_1(\psi, y_j) + \mathcal{O}(|x - y_j|), \quad d = 2,$$

$$\psi(x) = \frac{1}{4\pi|x - y_j|} L_0(\psi, y_j) + L_1(\psi, y_j) + \mathcal{O}(|x - y_j|), \quad d = 3.$$

Local self-adjoint extension are then given by

$$L_1(\psi, y_j) - \alpha L_0(\psi, y_j) = 0, \quad \alpha \in \mathbb{R};$$

the absence of interaction corresponds to $\alpha = \infty$, we refer again to



S. Albeverio, F. Gesztesy, R. Høegh-Krohn, H. Holden: Solvable Models in Quantum Mechanics, 2nd edition, Amer. Math. Soc., Providence, R.I., 2005.

Theorem

The *ground state* of $H_{\alpha, \Gamma}^N$ is uniquely maximized by a *N-regular polygon*.



P.E.: Necklaces with interacting beads: isoperimetric problems, in Proceedings of the “International Conference on Differential Equations and Mathematical Physics” (Birmingham 2006), AMS *Contemporary Mathematics Series*, vol. 412, Providence, R.I., 2006; pp. 141-149.

More results on spectral optimization will be given in the next lecture.

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- In contrast to Faber-Krahn-type results, the ground-state energy of leaky loops and point-interaction 'necklaces' is *maximized* by configurations of the maximum symmetry