Constrained quantum dynamics

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With thanks to all my collaborators

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- This motivates us to present an alternative model describing *'leaky' quantum graphs*, and their various generalizations.

Hall effect

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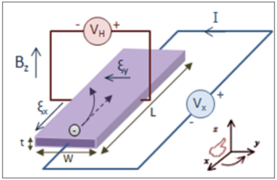

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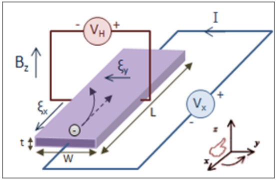

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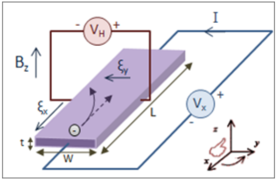

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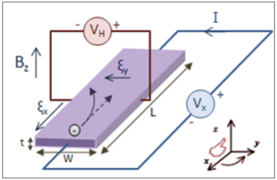

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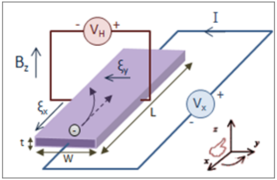

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In contrast to the 'usual' quantum Hall effect, its mechanism is not well understood; it is conjectured that it comes from *internal magnetization* in combination with the *spin-orbit interaction*.

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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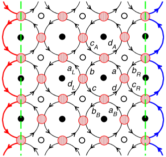

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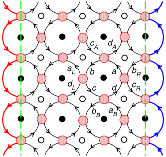

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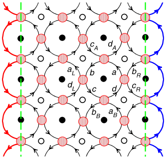

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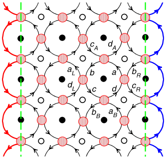

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Breaking the time-reversal invariance

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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

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

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Star graphs: spectrum and scattering

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

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*

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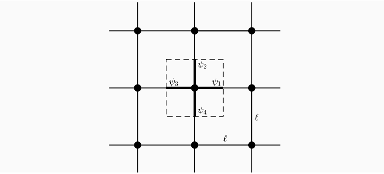
Let us look how this fact influences spectra of *periodic* quantum graphs.

Comparison of two lattices



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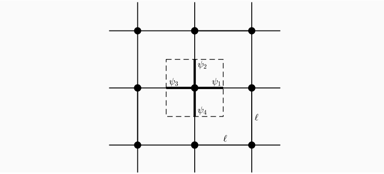

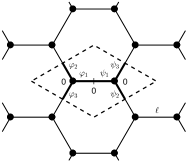

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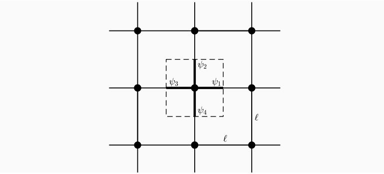

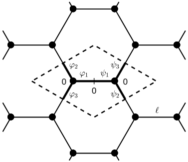

Spectral condition for the two cases are easy to derive,

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

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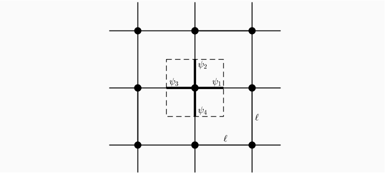

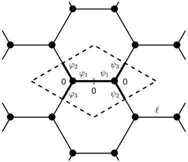

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and respectively

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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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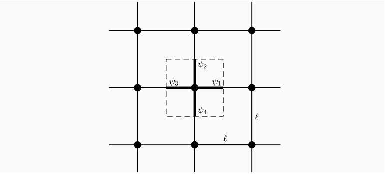

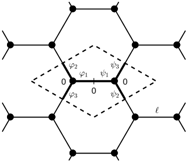

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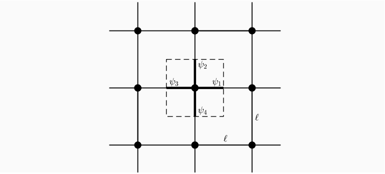
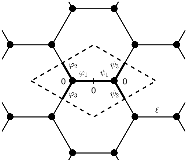
Comparison of two lattices





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

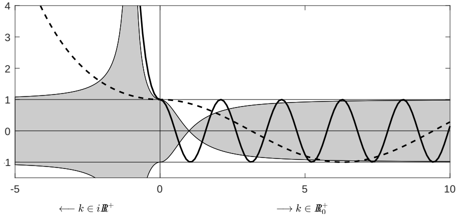
$$16i\,\mathrm{e}^{-i(\theta_1+\theta_2)}\,k^2\sin k\ell\left(3+6k^2-k^4+4d_\theta(k^2-1)+(k^2+3)^2\cos 2k\ell\right)=0\,,$$

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 $\ell = \frac{1}{4}$)



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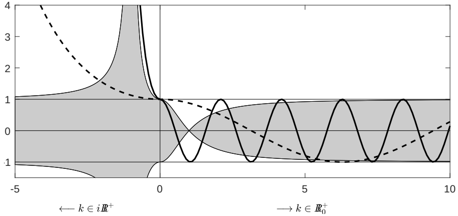

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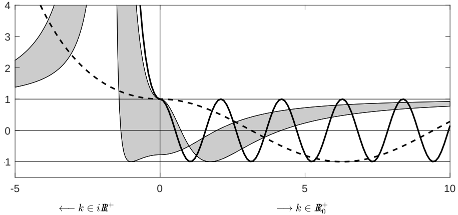

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Let us mention one more involved choice of the vertex coupling.

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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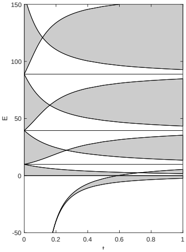

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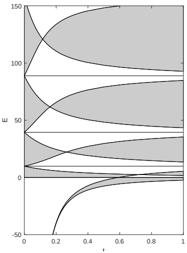

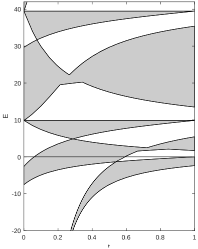

P.E., O. Turek, M. Tater: A family of quantum graph vertex couplings interpolating between different symmetries, *J. Phys. A: Math. Theor.* **51** (2018), 285301.

Another topic: band edges positions

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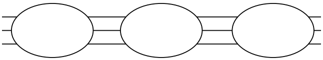

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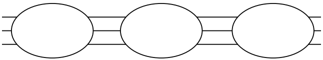

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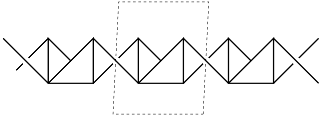

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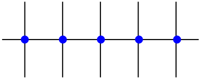

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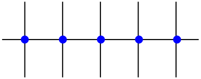

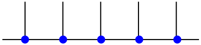

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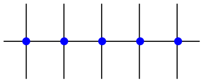

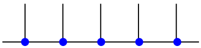

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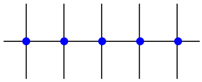

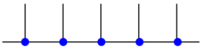

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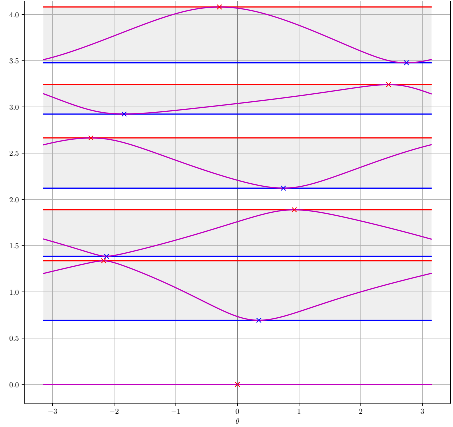
- and what about the dispersion curves?

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

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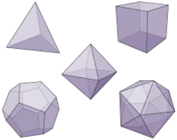

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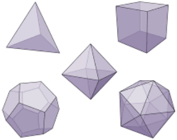

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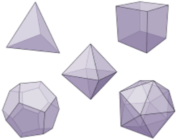

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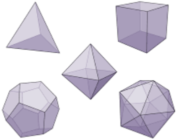

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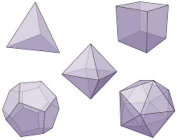

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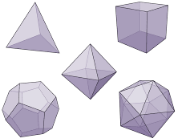

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P.E., J. Lipovský: Spectral asymptotics of the Laplacian on Platonic solids graphs, *J. Math. Phys.* **60** (2019), 122101

Another periodic graph model

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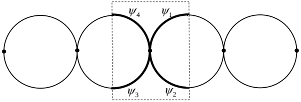
Let us look what this coupling influences graphs *periodic in one direction*. Consider again a *loop chain*, first *tightly connected*



The spectrum of the corresponding Hamiltonian looks as follows:

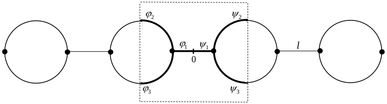
Theorem

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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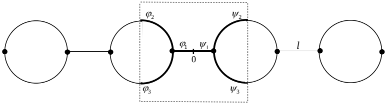

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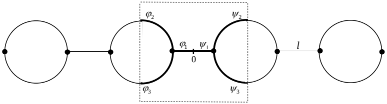

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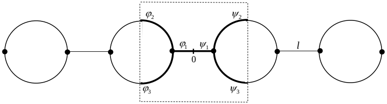

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- *The negative spectrum is contained in $(-\infty, -1)$ consisting of a single band if $\ell = \pi$, otherwise there is a pair of bands and $-3 \notin \sigma(H_\ell)$.*

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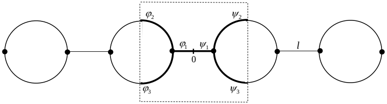

Theorem

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 $-3 \notin \sigma(H_\ell)$.*
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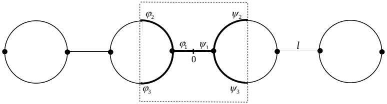

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- *The positive spectrum has infinitely many gaps.*
- $P_\sigma(H_\ell) := \lim_{K\to\infty} \frac{1}{K} |\sigma(H_\ell) \cap [0, K]| = 0$ *holds for any $\ell > 0$.*

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*, mentioned in Lecture III and introduced in

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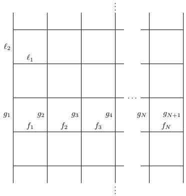
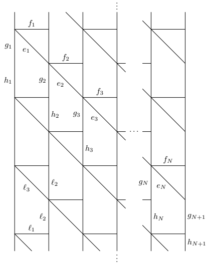
Note also that if we violate the mirror symmetry of the chain, we have instead $P_\sigma(H_0) = \frac{1}{2}$ independently of where exactly we place the vertex.

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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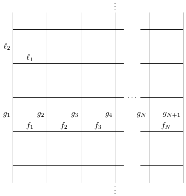

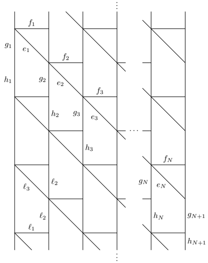

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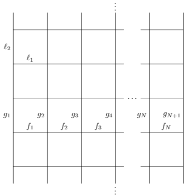

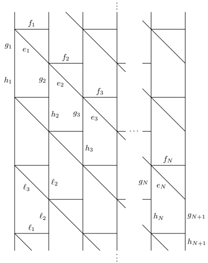

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This time we ask in which part of the ‘guide’ are the generalized eigenfunction *dominantly supported*

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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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* $k \to \infty$.

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

Leaky quantum graphs and their generalizations

Let us turn to the quantum graph *weakness* mentioned in the opening and try to find an alternative. The model we are going to examine now is based on singular Schrödinger operators that can formally written as

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We can regard them as *waveguides* of a sort, with a finite size of the transverse localization, and *building blocks* of more complicated structures.

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A natural way to define a singular Schrödinger operator on manifold of $\operatorname{codim}\Gamma = 1$ is to employ the appropriate quadratic form, namely

$$q_{\delta,\alpha}[\psi] := \|\nabla\psi\|^2_{L^2(\mathbb{R}^d)} - \alpha\|f|_\Gamma\|^2_{L^2(\Gamma)}$$

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Alternatively, one sometimes uses the symbol $-\Delta_{\delta,\alpha}$ for this operator; we will be mostly concerned with the situation where α is a *constant*.

The case $\operatorname{codim} \Gamma = 2$

This is more complicated but one can use again boundary conditions, appropriately modified. To begin with, for an infinite curve Γ referring to a map $\gamma : \mathbb{R} \to \mathbb{R}^3$ we have to assume in addition that there is a tubular neighbourhood of Γ which *does not intersect itself*

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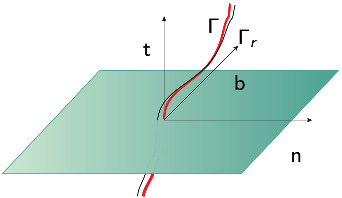
We employ *Frenet's frame* $(t(s), b(s), n(s))$ for Γ. Given $\xi, \eta \in \mathbb{R}$, we set $r = (\xi^2 + \eta^2)^{1/2}$ and define family of 'shifted' curves



$$\Gamma_r \equiv \Gamma_r^{\xi\eta} := \left\{ \gamma_r(s) \equiv \gamma_r^{\xi\eta}(s) := \gamma(s) + \xi b(s) + \eta n(s) \right\}$$

The case $\operatorname{codim}\Gamma = 2$, continued

The restriction of $f \in W^{2,2}_{\mathrm{loc}}(\mathbb{R}^3 \setminus \Gamma)$ to Γ_r is well defined for small r; we say that $f \in W^{2,2}_{\mathrm{loc}}(\mathbb{R}^3 \setminus \Gamma) \cap L^2(\mathbb{R}^3)$ belongs to Υ if the limits

$$\Xi(f)(s) := -\lim_{r \to 0} \frac{1}{\ln r} f \restriction_{\Gamma_r}(s),$$

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Note that absence of the interaction corresponds $\alpha = \infty$!

The case $\operatorname{codim}\Gamma = 2$, continued

The restriction of $f \in W^{2,2}_{\mathrm{loc}}(\mathbb{R}^3 \setminus \Gamma)$ to Γ_r is well defined for small r; we say that $f \in W^{2,2}_{\mathrm{loc}}(\mathbb{R}^3 \setminus \Gamma) \cap L^2(\mathbb{R}^3)$ belongs to Υ if the limits

$$\Xi(f)(s) := -\lim_{r\to 0} \frac{1}{\ln r} f\restriction_{\Gamma_r}(s),$$

$$\Omega(f)(s) := \lim_{r\to 0} \left[f\restriction_{\Gamma_r}(s) + \Xi(f)(s) \ln r \right],$$

exist a.e. in $\mathbb{R}$, are *independent* of the direction $\frac{1}{r}(\xi,\eta)$ in which they are taken, and define functions belonging to $L^2(\mathbb{R})$.

Then the corresponding singular Schrödinger operator $H_{\alpha,\Gamma}$ has the domain

$$\{\, g \in \Upsilon :\ 2\pi\alpha\Xi(g)(s) = \Omega(g)(s) \,\}$$

and acts as

$$-H_{\alpha,\Gamma} f = -\Delta f \quad \text{for} \quad x \in \mathbb{R}^3 \setminus \Gamma$$

Note that absence of the interaction corresponds $\alpha = \infty$!

Similarly one can treat the case $\operatorname{codim}\Gamma = 3$, replacing $\frac{1}{2\pi}\ln r$ by $\frac{1}{4\pi r}$, but this is more a mathematical exercise.

Spectral analysis: Birman-Schwinger principle

Theorem (Birman-Schwinger principle)

Let $H_\lambda := H_0 + \lambda V$ *on* $L^2(\mathbb{R}^d)$, *where* $H_0 = -\Delta$ *and* V *belongs to a suitable class. Then* $-\kappa^2$ *is an eigenvalue of* H_λ *for some* $\kappa > 0$ *if and only if the operator*

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For instance, if Γ is a *curve in the plane*, $H_{\alpha,\Gamma}$ has eigenvalue $-\kappa^2$ if and only if

$$\frac{\alpha}{2\pi}\int_\Gamma K_0(\kappa|\Gamma(s)-\Gamma(s')|)\phi(s')\,\mathrm{d}s' = \phi(s),$$

where s is the arc length of the curve Γ.

J.F. Brasche, P.E., Yu.A. Kuperin, P. Šeba: Schrödinger operators with singular interactions, *J. Math. Anal. Appl.* **184** (1994), 112–139.

Spectrum of $-\Delta_{\delta,\alpha}$

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On the other hand, the essential spectrum may change if the support Γ is non-compact. As an example, take a line in the plane and suppose that α is *constant and positive*; by separation of variables we find easily that $\sigma_{\mathrm{ess}}(-\Delta_{\delta,\alpha}) = [-\frac{1}{4}\alpha^2, \infty)$.

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The question about the *discrete spectrum* is more involved. Suppose first that interaction support is *finite*, $|\Gamma| < \infty$.

It is clear that $\sigma_{\mathrm{disc}}(-\Delta_{\delta,\alpha}) = \emptyset$ if the interaction is *repulsive*, $\alpha \leq 0$.

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$$\lambda(\alpha) = \big(C_\Gamma + o(1)\big)\, \exp\left(-\frac{4\pi}{\alpha|\Gamma|}\right) \quad \text{as} \quad \alpha|\Gamma| \to 0+$$

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J.-P. Antoine, F. Gesztesy, J. Shabani: Exactly solvable models of sphere interactions in quantum mechanics, *J. Phys. A: Mat. Gen.* **20** (1987), 3687–3712.

A δ-interaction supported by infinite curves

A geometrically induced discrete spectrum may exist even if Γ is infinite and $\inf \sigma_{\text{ess}}(-\Delta_{\delta,\alpha}) < 0$. Consider, for instance, a *non-straight, piecewise C^1-smooth curve* $\Gamma : \mathbb{R} \to \mathbb{R}^2$ parameterized by its arc length, $|\Gamma(s) - \Gamma(s')| \le |s - s'|$, assuming in addition that

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- Γ is *asymptotically straight*: there are $d > 0$, $\mu > \frac{1}{2}$ and $\omega \in (0,1)$ such that

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in the sector $S_\omega := \left\{(s, s') : \omega < \frac{s}{s'} < \omega^{-1}\right\}$

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Theorem

Under these assumptions, $\sigma_{\rm ess}(-\Delta_{\delta,\alpha}) = [-\frac{1}{4}\alpha^2, \infty)$ and $-\Delta_{\delta,\alpha}$ has at least one eigenvalue below the threshold $-\frac{1}{4}\alpha^2$.

P. Exner, T. Ichinose: *Geometrically induced spectrum in curved leaky wires*, J. Phys. **A34** (2001), 1439–1450.

Geometrically induced bound states, continued

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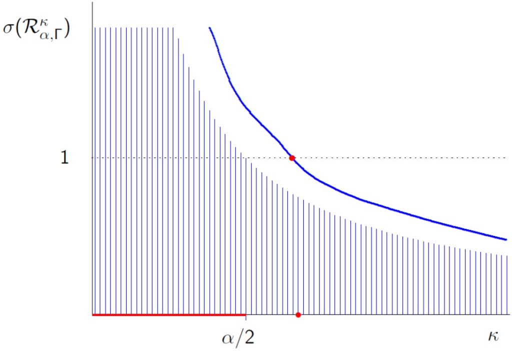
- The crucial observation is that – in view of the 2D free resolvent kernel properties – this perturbation is *sign definite* and *compact*.
- The best way to illustrate the main steps of the proof is to draw the spectrum of Birman-Schwinger operator in dependence on the spectral parameter κ.

Pictorial sketch of the proof



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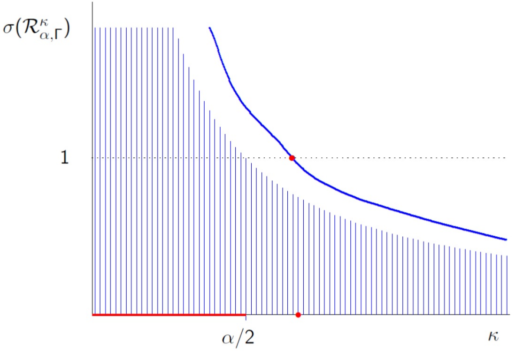

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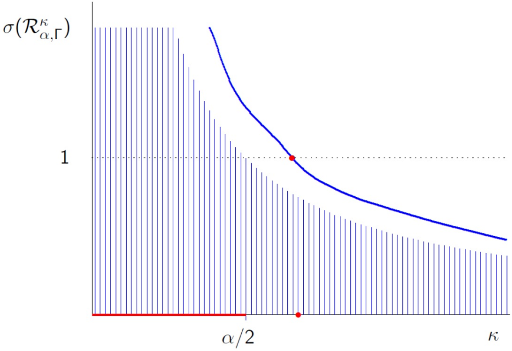

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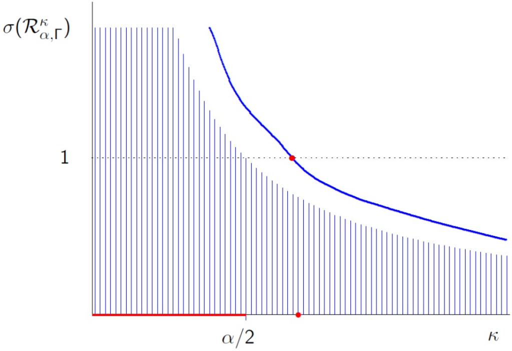

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- from the asymptotic straightness, the perturbation is *compact* so that the 'added' spectrum consists of eigenvalues at most
- the spectrum depends *continuously* on κ and *shrinks to zero* as $\kappa \to \infty$, hence there is a crossing *to the right* of $\frac{1}{2}\alpha$

Geometrically induced bound states, continued

- *Higher codimension*: for a *curve in* $\mathbb{R}^3$ which is *bent* or *locally deformed* but *asymptotically straight* we have an analogous result under slightly stronger regularity assumptions.

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- On the other hand, we have an example of a *conical surface* of an opening angle $\theta \in (0, \frac{1}{2}\pi)$ in $\mathbb{R}^3$, where for any constant $\alpha > 0$ we have $\sigma_{\text{ess}}(-\Delta_{\delta,\alpha}) = \mathbb{R}_+$ and an *infinite numbers of eigenvalues* below $-\frac{1}{4}\alpha^2$ accumulating at the threshold.

J. Behrndt, P.E., V. Lotoreichik: Schrödinger operators with δ-interactions supported on conical surfaces, *J. Phys. A: Math. Theor.* **47** (2014), 355202.

Geometrically induced bound states, continued

- Moreover, the above result remain valid for any *local deformation* of the conical surface. We also know the eigenvalue accumulation rate for conical layers

$$\mathcal{N}_{-\frac{1}{4}\alpha^2 - E}(-\Delta_{\delta,\alpha}) \sim \frac{\cot\theta}{4\pi}\,|\ln E|\,, \quad E \to 0+\,,$$

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- Implications for *more complicated Lipschitz partitions*: let $\tilde\Gamma \supset \Gamma$ holds in the set sense, then $H_{\alpha,\tilde\Gamma} \le H_{\alpha,\Gamma}$. If the essential spectrum thresholds are the same – which is often easy to establish – then $\sigma_{\rm disc}(H_{\alpha,\tilde\Gamma}) \neq \emptyset$ whenever the same is true for $\sigma_{\rm disc}(H_{\alpha,\Gamma})$

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$$V_\epsilon(x) = \begin{cases} 0 & v \notin \Sigma_\epsilon \\ -\frac{1}{\epsilon} V\left(\frac{u}{\epsilon}\right) & v \in \Sigma_\epsilon \end{cases}$$

In [E-Ichinose'01, loc.cit.] we proved the following convergence result:

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Point interaction approximation

The above approximation gives meaning to the δ interaction but it useless for computational purposes. To get a practical tool to solve the spectral problem for our operators, we replace the singular interaction supported by Γ by an *array $Y = \{y_j\}$ of point interactions*

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

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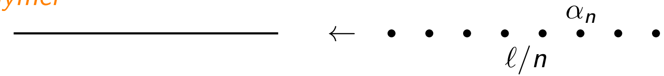
S. Albeverio, F. Gesztesy, R. Høegh-Krohn, H. Holden: Solvable Models in Quantum Mechanics, second edition, Amer. Math. Soc., Providence, R.I., 2005.

To guess how the coupling parameters of the point interaction should be chosen one can compare $H_{\alpha,\Gamma}$ for a straight Γ with the solvable model of a *straight-polymer*



Point interaction approximation, contd.

To get the same spectral threshold we need $\alpha_n = \alpha n$ which naturally means that individual point interactions get *weaker*. Hence we approximate $H_{\alpha,\Gamma}$ by point-interaction Hamiltonians H_{α_n,Y_n} with $\alpha_n = \alpha|Y_n|$, where $|Y_n| := \sharp Y_n$

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Theorem

Let a family $\{Y_n\}$ of finite sets $Y_n \subset \Gamma \subset \mathbb{R}^2$ be such that

$$\frac{1}{|Y_n|} \sum_{y \in Y_n} f(y) \to \int_\Gamma f \, \mathrm{d}m$$

holds for any bounded continuous $f : \Gamma \to \mathbb{C}$, together with technical conditions, then $H_{\alpha_n,Y_n} \to H_{\alpha,\Gamma}$ in the strong resolvent sense as $n \to \infty$.

P.E., K. Němcová: Leaky quantum graphs: approximations by point interaction Hamiltonians, *J. Phys.* **A36** (2003), 10173–10193.

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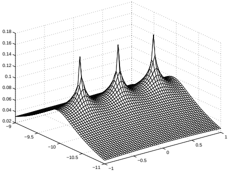

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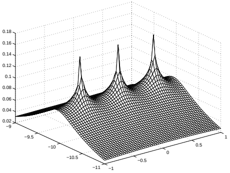

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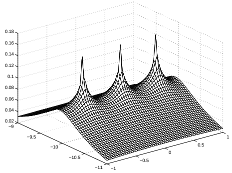

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- There is a trick: consider approximation of $\epsilon\Delta^2 - \Delta - \alpha\delta(x - \Gamma)$ and then take $\epsilon \to 0$; this gives a *norm-resolvent* convergence.

  J.F. Brasche, K. Ožanová: Convergence of Schrödinger operators, *SIAM J. Math. Anal.* **39** (2007), 281–297.

An application: scattering on leaky wires

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- It is expected that for strong coupling the states are *strongly transversally localized* and the motion would be *effectively one-dimensional*, while generally the *tunneling* may play role.

An example: a bottleneck curve

Recall a well-known physicist's trick to study *resonances* by exploring *spectral properties* of the problem cut to a finite length L and to look for *avoided crossings* in the L eigenvalue dependence.

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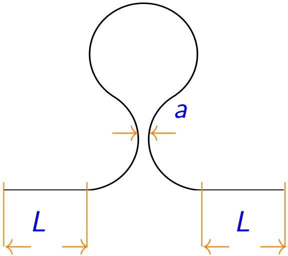

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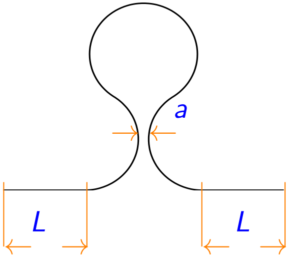

If Γ is a straight line, the transverse eigenfunction is $\mathrm{e}^{-\alpha|y|/2}$, hence the distance at which tunneling becomes significant is $\approx 4\alpha^{-1}$. In the example, we choose $\alpha = 1$.

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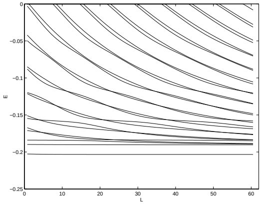

Wide bottleneck, $a = 5.2$

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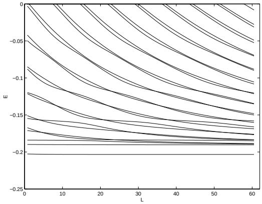

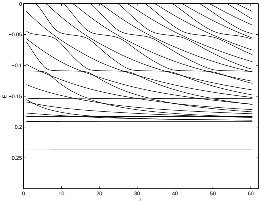

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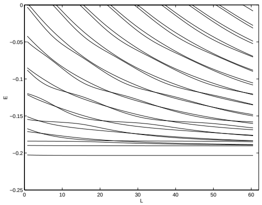

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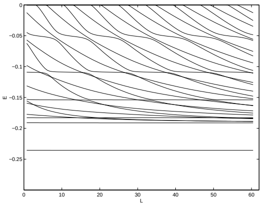

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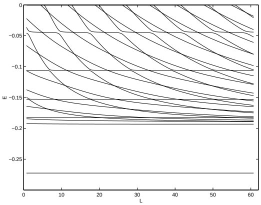

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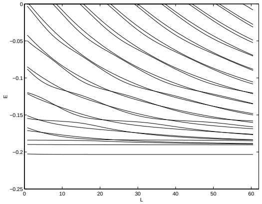

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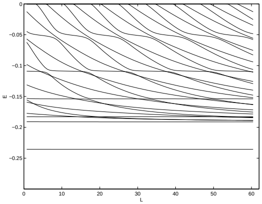

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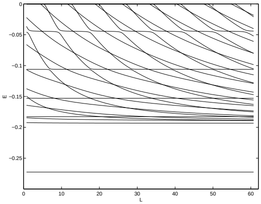

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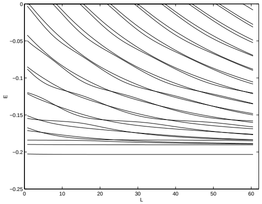

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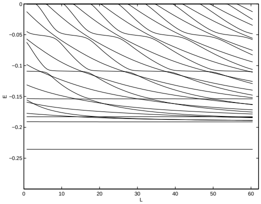

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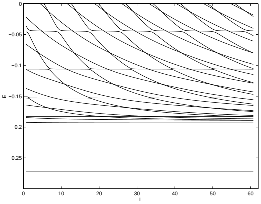

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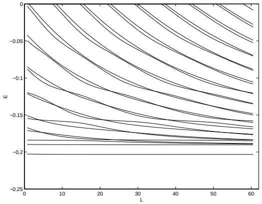

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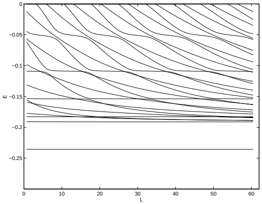

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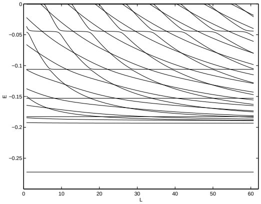

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