Constrained quantum dynamics

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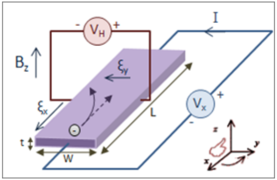
Some features of quantum graph models

Our encounter with quantum graphs revealed various properties of these models. In this lecture we focus on two of them:

- The first, which one may regard as their *advantage* is the multitude of the ways to choose a proper – self-adjoint – *vertex coupling*.
- This does not mean that 'exotic' couplings, different from Kirchhoff or δ, must describe the complicated structures we discussed in Lecture II; we may choose the coupling *ad hoc* to suit the physics of the effect we want to describe. We are going to discuss a class of such models.
- The other, which is rather a *disadvantage* comes from the fact that particles are supposed to be *strictly localized* at the graph edges. Should such a graph model, say, a network of actual semiconductor wires, we face the fact that the *quantum tunneling* between different part of the graph is *neglected* which, depending of the geometry of the problem, may not be realistic.
- This motivates us to present an alternative model describing *'leaky' quantum graphs*, and their various generalizations.

Hall effect

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



Source: Wikipedia

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

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

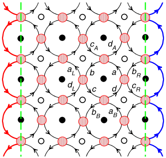
However, in ferromagnetic material one can observe a similar behavior also in the *absence of external magnetic field* – being labeled *anomalous*.

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

Modeling anomalous Hall effect

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

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



Source: the cited paper

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

Breaking the time-reversal invariance

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

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

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

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

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

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

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

Star graphs: spectrum and scattering

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

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

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

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

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

The vertex parity enters the game

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

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

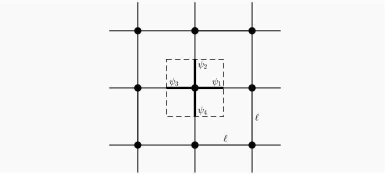
in particular, for $N = 3, 4$, respectively, we get

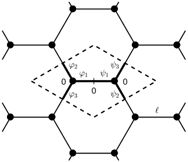
$$\frac{1+\eta}{1+\eta+\eta^2} \begin{pmatrix} -\frac{\eta}{1+\eta} & 1 & \eta \\ \eta & -\frac{\eta}{1+\eta} & 1 \\ 1 & \eta & -\frac{\eta}{1+\eta} \end{pmatrix} \quad \text{and} \quad \frac{1}{1+\eta^2} \begin{pmatrix} -\eta & 1 & \eta & \eta^2 \\ \eta^2 & -\eta & 1 & \eta \\ \eta & \eta^2 & -\eta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

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

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

Comparison of two lattices





Spectral condition for the two cases are easy to derive,

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

and respectively

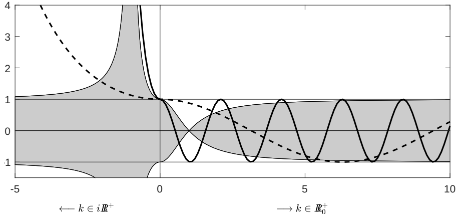
$$16i\,\mathrm{e}^{-i(\theta_1+\theta_2)}\,k^2\sin k\ell\left(3+6k^2-k^4+4d_\theta(k^2-1)+(k^2+3)^2\cos 2k\ell\right)=0\,,$$

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

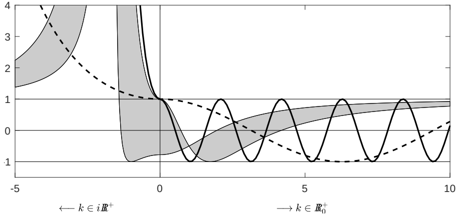
P.E., M. Tater: Quantum graphs with vertices of a preferred orientation, *Phys. Lett.* **A382** (2018), 283–287.

A picture is worth of thousand words

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



and



Comparison summary

Some features are common:

- the number of open gaps is *always infinite*
- the gaps are centered around the flat bands except the lowest one
- for some values of ℓ a band may *degenerate*
- the negative spectrum is *always nonempty*, the gaps become *exponentially narrow* around star graph eigenvalues as $\ell \to \infty$

But the *high energy behavior* of these lattices is *substantially different*:

- the spectrum is dominated by *bands* for square lattices
- it is dominated by *gaps* for hexagonal lattices

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

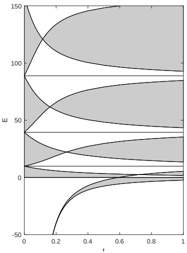
Let us mention one more involved choice of the vertex coupling.

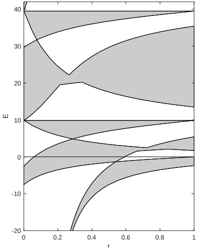
An interpolation

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

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

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





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

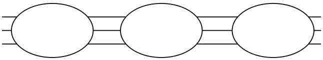
Another topic: band edges positions

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

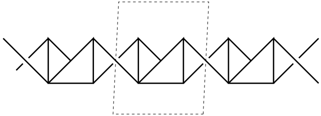
J.M. Harrison, P. Kuchment, A. Sobolev, B. Winn: On occurrence of spectral edges for periodic operators inside the Brillouin zone, *J. Phys. A: Math. Theor.* **40** (2007), 7597–7618.

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

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



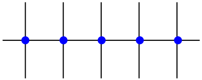
The number of connecting edges had to be $N \geq 2$. An example:

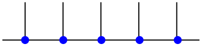


Band edges, continued

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

However, we did it under that assumption that the system is *invariant w.r.t. time reversal*. To show that this assumption was essential consider a *comb-shaped graph* with our non-invariant coupling at the vertices

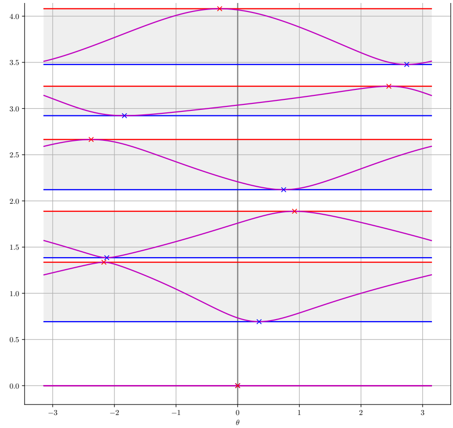




Its analysis shows:

- *two-sided comb* is *transport-friendly*, bands dominate
- *one-sided comb* is *transport-unfriendly*, gaps dominate
- sending the one side edge lengths to zero in a two-sided comb *does not yield* one-sided comb transport
- and what about the dispersion curves?

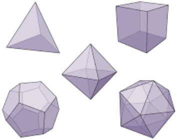
Two-sided comb: dispersion curves



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

Discrete symmetry: Platonic solid graphs

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



Source: Wikipedia Commons

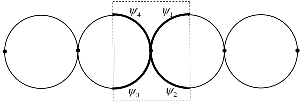
and assume the described coupling in the vertices. The corresponding spectra are discrete but their *high-energy behavior differs:*

- for tetrahedron, cube, icosahedron, and dodecahedron the square roots of ev's *approach integer multiples of* π with an $\mathcal{O}(k^{-1})$ error
- *octahedron* also has such eigenvalues, but in addition it has *two other series:* those behaving as $k = 2\pi n \pm \frac{2}{3}\pi$ for $n \in \mathbb{Z}$, and as $k = \pi n + \frac{1}{2}\pi$ with an $\mathcal{O}(k^{-2})$ error
- no such distinction exists for more common couplings such as δ

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

Another periodic graph model

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



The spectrum of the corresponding Hamiltonian looks as follows:

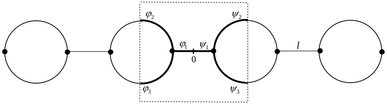
Theorem

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

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

A loosely connected chain

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



Theorem

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

- *Any non-negative integer is an eigenvalue of infinite multiplicity.*
- *Away of the non-negative integers the spectrum is absolutely continuous having a band-and-gap structure.*
- *The negative spectrum is contained in $(-\infty, -1)$ consisting of a single band if $\ell = \pi$, otherwise there is a pair of bands and $-3 \notin \sigma(H_\ell)$.*
- *The positive spectrum has infinitely many gaps.*
- $P_\sigma(H_\ell) := \lim_{K\to\infty} \frac{1}{K} |\sigma(H_\ell) \cap [0, K]| = 0$ *holds for any $\ell > 0$.*

The limit $\ell \to 0+$

The quantity $P_\sigma(H_\ell)$ in the last claim of the theorem is the *probability of being in the spectrum*, mentioned in Lecture III and introduced in

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

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

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

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

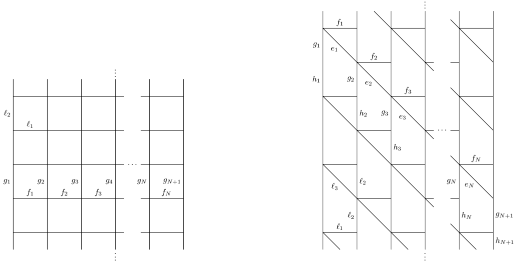
We have, however, obviously $P_\sigma(H_0) = 1$, hence our example shows that the said convergence may be *rather nonuniform!*

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

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

One more example: transport properties

Consider strips cut of the following two types of lattices:



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

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

Transport properties, continued

Theorem

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

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

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

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

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

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

$$H_{\alpha,\Gamma} = -\Delta - \alpha\delta(x-\Gamma), \quad \alpha > 0,$$

in $L^2(\mathbb{R}^d)$, where Γ is a graph understood as a subset of $\mathbb{R}^d$.

Why is it interesting? One can expect that a particle in a state from the *negative spectral subspace* will remain *localized close to* Γ, the closer the larger is the coupling strength α, and at the same time, the whole $\mathbb{R}^d$ is accessible to it, so it can tunnel from one point to another.

In fact, the dimension of Γ is not that important – what matters is rather its *codimension* – and we begin with the simplest situation where Γ is a *smooth manifold* in $\mathbb{R}^d$ having in mind primarily three important cases:
curves in $\mathbb{R}^2$, surfaces in $\mathbb{R}^3$, and curves in $\mathbb{R}^3$

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

A δ-interaction supported by a manifold

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

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

with the domain $H^1(\mathbb{R}^d)$ and to use the first representation theorem to define a unique self-adjoint operator $H_{\alpha,\Gamma}$; it is enough that Γ is *Lipschitz*

J. Behrndt, P.E., M. Holzmann, V. Lotoreichik: Approximation of Schrödinger operators with δ-interactions supported on hypersurfaces, *Math. Nachr.* **290** (2017), 1215–1248.

If Γ is a *smooth manifold* with $\operatorname{codim}\Gamma = 1$ one can alternatively use boundary conditions: $H_{\alpha,\Gamma}$ acts as $-\Delta$ on functions from $H^2_{\mathrm{loc}}(\mathbb{R}^d \setminus \Gamma)$, which are continuous and exhibit a normal-derivative jump,

$$\frac{\partial\psi}{\partial n}(x)\bigg|_+ - \frac{\partial\psi}{\partial n}(x)\bigg|_- = -\alpha(x)\psi(x)$$

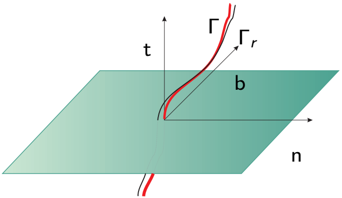
This explains the formal expression as describing the *attractive δ-interaction* of strength $\alpha(x)$ perpendicular to Γ at the point x.

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*

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 $\mathrm{codim}\,\Gamma = 2$, 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 $\mathrm{codim}\,\Gamma = 3$, 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

$$K_\kappa := |V|^{1/2}(H_0 + \kappa^2)^{-1} V^{1/2}$$

has eigenvalue $-\lambda^{-1}$, and moreover, their multiplicities are the same.

For singular Schrödinger operators we consider here this makes no sense, but we have an *analogous result* in which the above K_κ is replaced by an *integral operator* on $L^2(\Gamma)$ with the kernel $(H_0 + \kappa^2)^{-1}(\cdot,\cdot)$.

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

The spectrum is determined both by the *geometry of* Γ and the coupling function α, in particular, by its *sign*.

If Γ is *compact*, it is easy to see that $\sigma_{\mathrm{ess}}(-\Delta_{\delta,\alpha}) = \mathbb{R}_+$.

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 $\sigma_{\mathrm{ess}}(-\Delta_{\delta,\alpha}) = [-\frac{1}{4}\alpha^2, \infty)$.

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*, $\alpha \leq 0$.

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

On the other hand, the existence of a negative discrete spectrum for an attractive coupling is *dimension dependent*.

Consider for simplicity a constant α. For $d = 2$ bound states then exist whenever $|\Gamma| > 0$, in particular, we have a *weak-coupling expansion*

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

S. Kondej, V. Lotoreichik: Weakly coupled bound state of 2-D Schrödinger operator with potential-measure, *J. Math. Anal. Appl.* **420** (2014), 1416–1438.

On the other hand, for $d = 3$ the singular coupling must exceed a critical value. As an example, let Γ be a sphere of radius $R > 0$ in $\mathbb{R}^3$, then we have

$$\sigma_{\rm disc}(H_{\alpha,\Gamma}) \neq \emptyset \quad \text{if and only if} \quad \alpha R > 1,$$

and the same obviously holds in dimensions $d > 3$.

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

- $|\Gamma(s) - \Gamma(s')| \ge c|s - s'|$ holds for some $c \in (0,1)$
- Γ is *asymptotically straight*: there are $d > 0$, $\mu > \frac{1}{2}$ and $\omega \in (0,1)$ such that

$$1 - \frac{|\Gamma(s) - \Gamma(s')|}{|s - s'|} \le d\left[1 + |s + s'|^{2\mu}\right]^{-1/2}$$

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

Theorem

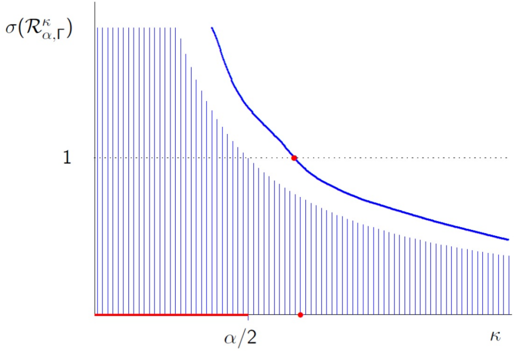
Under these assumptions, $\sigma_{\text{ess}}(-\Delta_{\delta,\alpha}) = [-\frac{1}{4}\alpha^2, \infty)$ and $-\Delta_{\delta,\alpha}$ has at least one eigenvalue below the threshold $-\frac{1}{4}\alpha^2$.

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

Geometrically induced bound states, continued

- The result is obtained via (generalized) Birman-Schwinger principle regarding the bending a *perturbation of the straight line*.
- 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



- in the straight case $\sigma(\mathcal{R}^\kappa_{\alpha,\Gamma_0}) = [0, \frac{1}{2}\alpha]$ is checked directly
- using a trial function one proves that $\sup \sigma(\mathcal{R}^\kappa_{\alpha,\Gamma}) > \frac{1}{2}\alpha$
- 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.

  P. Exner, S. Kondej: Curvature-induced bound states for a δ interaction supported by a curve in $\mathbb{R}^3$, *Ann. Henri Poincaré* **3** (2002), 967–981.

- *Higher dimensions*: here the situation is more complicated; for *smooth curved surfaces* $\Gamma \subset \mathbb{R}^3$ an analogous result is proved in the strong coupling asymptotic regime, $\alpha \to \infty$, only.

  P. Exner, S. Kondej: Bound states due to a strong δ interaction supported by a curved surface, *J. Phys. A: Math. Gen.* **36** (2003), 443–457.

- 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

$$\mathcal{N}_{-\frac14\alpha^2-E}(-\Delta_{\delta,\alpha}) \sim \frac{\cot\theta}{4\pi}\,|\ln E|\,, \quad E\to 0+\,,$$

  and a similar formula holds for *noncylindrical* cones.

V. Lotoreichik, T. Ourmières-Bonafos: On the bound states of Schrödinger operators with δ-interactions on conical surfaces, *Comm. PDE* **41** (2016), 999–1028.

T. Ourmières-Bonafos, K. Pankrashkin: Discrete spectrum of interactions concentrated near conical surfaces, *Appl. Anal.* **97** (2018) 1628–1649.

- On the other hand, the result is again dimension-dependent: for a conical surface in $\mathbb{R}^d$, $d>3$, we have $\sigma_{\rm disc}(-\Delta_{\delta,\alpha})=\emptyset$
- 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 $\sigma_{\rm disc}(H_{\alpha,\tilde\Gamma})\ne\emptyset$ whenever the same is true for $\sigma_{\rm disc}(H_{\alpha,\Gamma})$

Approximation of the singular interaction

The question naturally arises about the *meaning* of such models. To address it, let Γ be a C^4 smooth curve in $\mathbb{R}^2$ with a strip neighborhood which *does not intersect itself*, parametrized by the *locally orthogonal coordinates* s, u mentioned in Lecture I.

Given a fixed function $V \in L^\infty(-1,1)$ we consider potentials with the support in the strip $\Sigma_\epsilon := \{(s,u) :\ |u| < \epsilon\}$ given by

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

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

$$-\Delta + V_\epsilon \to H_{\alpha,\Gamma} \quad \text{in the norm-resolvent sense as } \epsilon \to 0,$$

where $\alpha := \int_{-1}^{1} V(u)\,\mathrm{d}u$. This claim can be substantially generalized as shown in [Behrndt-E-Holzmann-Lotoreichik'17, loc.cit.], where

- Γ is a *C^2-smooth orientable surface*, $\operatorname{codim}\Gamma = 1$, in $\mathbb{R}^n$, $n \geq 2$,
- the 'target' coupling strength α is *any L^∞ function* on Γ, modulo some technical assumptions.

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*

We employ generalized boundary values at $y_j \in Y$ using the expansion

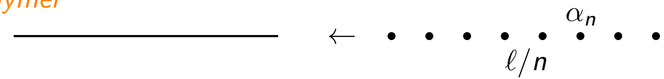
$$\psi(x) = -\frac{1}{2\pi} \log|x - y_j|\, L_0(\psi, y_j) + L_1(\psi, y_j) + \mathcal{O}(|x - y_j|)$$

a *local* self-adjoint extension is then given by

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

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 $|Y_n| := \sharp Y_n$. Then we have

Theorem

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

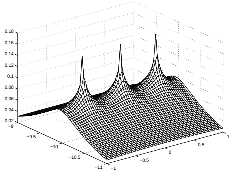
$$\frac{1}{|Y_n|} \sum_{y\in Y_n} f(y) \to \int_\Gamma f \, \mathrm{d}m$$

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.

Point interaction approximation: remarks

- The limit is a *homogenization of a sort*. Eigenfunctions of the approximating operator which look as



  will in the limit produce the corresponding eigenfunction of $H_{\alpha,\Gamma}$, *continuous and locally bounded* at the curve Γ having a *jump of the normal derivative* there (the convergence is *slower than $\mathcal{O}(n^{-1})$*).
- Similarly one can approximate *surfaces* Γ by *3D point interactions*.

  J.F. Brasche, R. Figari, A. Teta: Singular Schrödinger operators as limits of point interaction Hamiltonians, *Potential Anal.* **8** (1998), 163–178.
- 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

To give an example how one can use the approximation, consider the *scattering problem* on a leaky graph with *semi-infinite 'leads'*. What is known and expected in this case?

- *What is the 'free' operator?* Obviously $-\Delta$ is not a good candidate, rather $H_{\alpha,\Gamma}$ for a straight line Γ; recall that we are particularly interested in energy interval $(-\frac{1}{4}\alpha^2, 0)$, i.e. the one-dimensional transport of states *laterally bound to* Γ.
- *Existence and completeness* was proved if the external leads belong to a line; there is also a general existence result.

P.E., S. Kondej: Scattering by local deformations of a straight leaky wire, *J. Phys.* **A38** (2005), 4865–4874.

J. Dittrich: Scattering of particles bounded to infinite planar curve, *Rev. Math. Phys.* **32** (2020), 2050029.

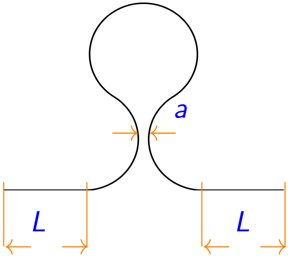
- It is expected that for strong coupling the states are *strongly transversally localized* and the motion would be *effectively one-dimensional*, while generally the *tunneling* may play role.

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.

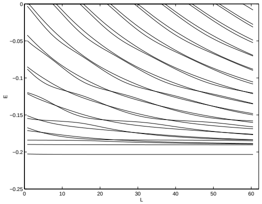
G.A. Hagedorn, B. Meller: Resonances in a box, *J. Math. Phys.* **41** (2000), 103–117.

Consider a straight line deformation which shaped as an open loop with a bottleneck the width a of which we will vary

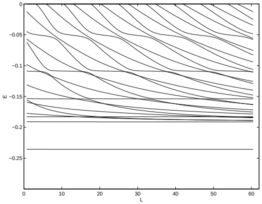


If Γ is a straight line, the transverse eigenfunction is $\mathrm{e}^{-\alpha|y|/2}$, hence the distance at which tunneling becomes significant is $\approx 4\alpha^{-1}$. In the example, we choose $\alpha = 1$.

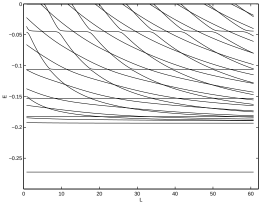
An example: a bottleneck curve



Wide bottleneck, $a = 5.2$



Narrow bottleneck, $a = 2.9$



Even narrower one, $a = 1.9$

We see that if the bottleneck width is small enough, the system exhibits *resonances*, obviously caused by *tunneling* between adjacent parts.

Those are absent in the 'conventional' quantum graph where the curve is *equivalent to a straight line*, and this cannot be changed even if we add a *curvature-induced potential*, say, $-\frac{1}{4}\gamma(s)^2$; to see that, it is enough to 'flip' one half of the curve.

What to bring home from Lecture IV

- Also some *'unusual' vertex couplings* may be of physical interest.
- Graphs can provide example warning against *risks* of 'folklore' methods of using PDEs.
- Schrödinger operators with singular interactions provided us with *alternative ways* to describe guided dynamics.
- In this framework again, *geometry* can determine *spectral properties*.
- We have *efficient computational tools* to treat these problems.
- Leaky quantum structures reveal effects *inaccessible within more conventional models*.