Constrained quantum dynamics

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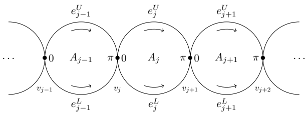
Magnetic effects and soft waveguides

Of the numerous extensions of the topics discussed in the previous lectures we are going to discuss here two:

- The first one concerns the effects that a *magnetic field* can have on a constrained motion. They are numerous. For instance, under a homogeneous field periodic graphs can have *flat bands only*.
- One the magnetic field is inhomogenous, the result can be even more spectacular, for instance, the spectrum may have a *fractal character*.
- Likewise, interesting magnetic effects occur in *leaky graphs*, e.g., the field can change the *effective size* of the graph entering the Weyl asymptotics, or a loop with a strong enough coupling may exhibit *persistent currents*.
- In infinite graphs even an *Aharonov-Bohm field* that vanishes everywhere except one point may alter the spectrum dramatically.
- We will also mention a model of *soft waveguides* which reflects the deficiencies of both the hard-wall tubes and leaky graphs making use of guiding effects of *finite-width potential ditches*.

A magnetic ring chain

Our first example illustrating that a magnetic field is able to *change the spectral properties fundamentally* concerns the *ring chain* discussed in Lecture III; now we suppose that is exposed to a field, in general inhomoheneous, *perpendicular to the graph plane*.



The Hamiltonian is now the *magnetic Laplacian*, $\psi_j \mapsto -\mathcal{D}^2\psi_j$ on each graph link, where $\mathcal{D} := -i\nabla - A$, and for we again assume *δ-coupling* in the vertices, i.e. the domain consists of functions from $H^2_{\rm loc}(\Gamma)$ satisfying

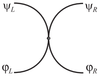
$$\psi_i(0) = \psi_j(0) =: \psi(0)\,, \quad i,j = 1,\dots,n\,, \quad \sum_{i=1}^{n} \mathcal{D}\psi_i(0) = \alpha\,\psi(0)\,,$$

V. Kostrykin, R. Schrader: Quantum wires with magnetic fluxes, *Commun. Math. Phys.* **237** (2003), 161–179.

Here $\alpha \in \mathbb{R}$ is again the coupling constant and we have $n = 4$. In fact, the vector potentials cancel and we get the same condition as before.

Floquet analysis of the fully periodic case

Consider first the case when the field is *homogenous*, $A_j = A,\ j \in \mathbb{Z}$. As before the solution comes from analysis of the *basic cell* of the chain,



We use a modified Ansatz $\psi_L(x) = \mathrm{e}^{-iAx}(C_L^+ \mathrm{e}^{ikx} + C_L^- \mathrm{e}^{-ikx})$ for $x \in [-\pi/2, 0]$ and energy $E := k^2 \neq 0$, and similarly for the other three components; for $E < 0$ we put instead $k = i\kappa$ with $\kappa > 0$.

The functions are again matched through *(a) the δ-coupling* and *(b) Floquet conditions*. Using the function $\eta(k) := 4\cos k\pi + \frac{\alpha}{k}\sin k\pi$, we can write now the spectral condition as

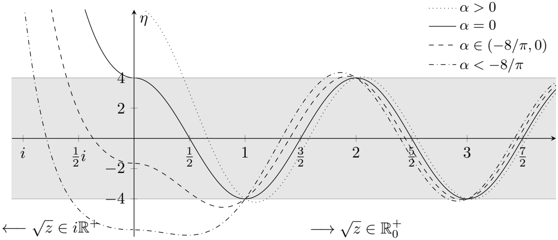
$$|\eta(k)| \leq 4|\cos A\pi|\,;$$

the difference due to the magnetic field presence is at the right-hand side; note that it is the *fractional part* of A which matters.

It is illustrative to show the solutions in the graphical form.

In picture: determining the spectral bands

It is easy to see that the degenerate bands referring to *Dirichlet eigenvalues* are not affected to the magnetic field; the other bands can be derived from the picture we have seen before,



however, vertically the shaded strip *shrinks* for a *non-integer A* to the interval $[-4|\cos A\pi|, 4|\cos A\pi|]$, in particular, to a *line* for $A - \frac{1}{2} \in \mathbb{Z}$.

Conseuently, in the latter case the chain spectrum consists of *infinitely degenerate eigenvalues* only, or *flat bands* as physicists would say, and elementary eigenfunctions are supported by *pairs of adjacent loops*.

Making it a little more complicated

It is relatively easy to deal with *local perturbations*. In a similar way we dealt with a *bent chain* we can treat a variation of A in a single ring, $A = \{\dots, A, A_1, A \dots\}$. It may or may not give rise to a discrete spectrum; we have a single simple eigenvalue in each gap provided

$$\frac{|\cos A_1\pi|}{|\cos A\pi|} > 1,$$

i.e. 'closer the non-magnetic case', otherwise spectrum does not change.

P.E., Stepan Manko: Spectral properties of magnetic chain graphs, *Ann. H. Poincaré* **18** (2017), 929–953.

Global changes are more interesting. Suppose that the field varies *linearly* along the chain, $A_j = \mu j + \theta$ for some $\mu, \theta \in \mathbb{R}$ and every $j \in \mathbb{Z}$.

You may say, that in nature one never meets a (globally) linear magnetic field. As a possible excuse, let me quote Bratelli and Robinson:

... while the experimentalist might collect all his data between breakfast and lunch in a small cluttered laboratory, his theoretical colleagues interpret those results in terms of isolated systems moving eternally in an infinitely extended space. The validity of such idealizations is the heart and soul of theoretical physics and has the same fundamental significance as the reproducibility of experimental data.

A more practical point of view

One can also say: it is the *bridge at which mathematics and physics meet*, at least since Newton times.

In fact, the unbounded character of the sequence $\{A_j\}$ need not bother us as it is not essential. The point is that, as we noted already, from the spectral point of view only the *fractional part of each A_j matters.*

The reason is that our operator – which we denote as $-\Delta_{\alpha,A}$ a given $\alpha \in \mathbb{R}$ and $A = \{A_j\} \subset \mathbb{R}$ – is *unitarily equivalent* to $-\Delta_{\alpha,A'}$ with $A'_j = A_j + n$ with $n \in \mathbb{Z}$ by the operator acting as $\psi_j(x) \mapsto \psi_j(x)\,\mathrm{e}^{-inx}$; a physicist would call it a *gauge transformation*.

This simplifies the analysis in the case when the *slope μ is rational*. Indeed, is such a situation we can assume without loss of generality that the sequence $\{A_j\}$ is *periodic* and solve the problem using the Floquet method similarly as we did that for a constant A.

Results of Floquet analysis in the rational case

Theorem

Let $A_j = \mu j + \theta$ for some $\mu, \theta \in \mathbb{R}$ and every $j \in \mathbb{Z}$. Then for the spectrum $\sigma(-\Delta_{\alpha,A})$ the following holds:

(a) *If $\mu, \theta \in \mathbb{Z}$ and $\alpha = 0$, then $\sigma_{ac}(-\Delta_{\alpha,A}) = [0, \infty)$ and $\sigma_{pp}(-\Delta_{\alpha,A}) = \{n^2 |\, n \in \mathbb{N}\}$*

(b) *If $\alpha \neq 0$ and $\mu = p/q$ with p, q relatively prime, $\mu j + \theta + \frac{1}{2} \notin \mathbb{Z}$ for all $j = 0, \dots, q-1$, then $-\Delta_{\alpha,A}$ has infinitely degenerate ev's $\{n^2 |\, n \in \mathbb{N}\}$ interlaced with an ac part consisting of q-tuples of closed intervals*

(c) *If the situation is as in (b) but $\mu j + \theta + \frac{1}{2} \in \mathbb{Z}$ holds for some $j = 0, \dots, q-1$, then the spectrum $\sigma(-\Delta_{\alpha,A})$ consists of infinitely degenerate eigenvalues only, the Dirichlet ones plus q distinct others in each interval $(-\infty, 1)$ and $\big(n^2, (n+1)^2\big)$.*

P.E., D. Vašata: Cantor spectra of magnetic chain graphs, *J. Phys. A: Math. Theor. 50* (2017), 165201.

Duality

The case of an *irrational* μ requires a different approach.

The idea is to rephrase our *differential operator* problem of the metric graph in term of a *difference equation*, as proposed in the 1980's by physicists, Alexander and de Gennes, followed by mathematicians.

It is particularly simple if the graph in question is *equilateral* like in our example. We consider $\mathfrak{K} := \{k \colon \mathrm{Im}\, k \geq 0 \wedge k \notin \mathbb{Z}\}$ to exclude Dirichlet ev's and seek the spectrum through solution of $(-\Delta_{\alpha,A} - k^2)\binom{\psi(x,k)}{\varphi(x,k)} = 0$

This leads to the difference equation

$$2\cos(A_j\pi)\psi_{j+1}(k) + 2\cos(A_{j-1}\pi)\psi_{j-1}(k) = \eta(k)\psi_j(k)\,, \quad k \in \mathfrak{K}\,,$$

where $\psi_j(k) := \psi(j\pi, k)$ and $\eta(k) := 4\cos k\pi + \frac{\alpha}{k}\sin k\pi$ as above, amended by $\eta(k) = 4 + \alpha\pi$ for $k = 0$.

What is important, this is a two-way correspondence; we can *reconstruct* the solution of the original problem from that of the difference one.

Duality, continued

Specifically, we have

$$\begin{pmatrix} \psi(x,k) \\ \varphi(x,k) \end{pmatrix} = \mathrm{e}^{\mp iA_j(x-j\pi)} \Big[\psi_j(k) \cos k(x-j\pi)$$
$$+ (\psi_{j+1}(k)\mathrm{e}^{\pm iA_j\pi} - \psi_j(k)\cos k\pi) \frac{\sin k(x-j\pi)}{\sin k\pi} \Big], \quad x \in (j\pi, (j+1)\pi),$$

and in addition, the function on the left-hand side belongs to $L^p(\Gamma)$ if and only if $\{\psi_j(k)\}_{j\in\mathbb{Z}} \in \ell^p(\mathbb{Z})$ holds with $p \in \{2, \infty\}$.

This relates weak solutions of the two problems but we can do better:

Theorem

For any interval $J \subset \mathbb{R} \setminus \sigma_D$, the operator $(-\Delta_{\alpha,A})_J$ is unitarily equivalent to the pre-image $\eta^{(-1)}\big((L_A)_{\eta(J)}\big)$, where L_A is the operator on $\ell^2(\mathbb{Z})$ acting as $(L_A\varphi)_j = 2\cos(A_j\pi)\varphi_{j+1} + 2\cos(A_{j-1}\pi)\varphi_{j-1}$.

K. Pankrashkin: Unitary dimension reduction for a class of self-adjoint extensions with applications to graph-like structures, *J. Math. Anal. Appl.* **396** (2012), 640–655.

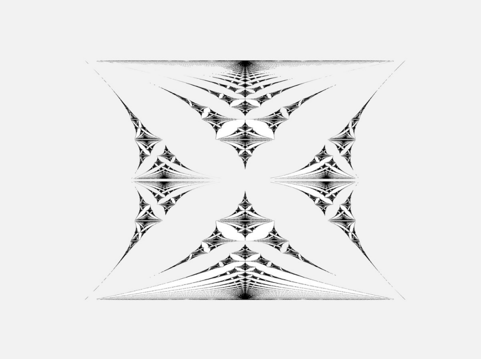
Another way to rephrase the problem

Let me recall the well-known *almost Mathieu equation*

$$u_{n+1} + u_{n-1} + \lambda \cos(2\pi\mu n + \theta))u_n = \epsilon u_n$$

in the *critical case*, $\lambda = 2$, also called *Harper equation*

The spectrum of the corresponding difference operator $H_{\mu,2,\theta}$, independent of θ, as a function of μ is the well-known *Hofstadter butterfly*



Source: Fermat's Library

The Ten Martini Problem

If $\mu \in \mathbb{Q}$, the spectrum of $H_{\mu,2,\theta}$ is easily seen to be absolutely continuous and of the band-gap type.

For $\mu \notin \mathbb{Q}$ the problem is much harder. Its *Cantor structure* was conjectured – under the name proposed by B. Simon – but it took two decades to achieve the solution:

A. Avila, S. Jitomirskaya: The Ten Martini Problem, *Ann. Math.* **170** (2009), 303–342.

Theorem

For any $\mu \notin \mathbb{Q}$, the spectrum of $H_{\mu,2,\theta}$ does not depend on θ and it is a Cantor set (i.e., having no interior points) of Lebesgue measure zero.

N.B.: Such a behavior was anticipated in physics half a century ago,

M.Ya. Azbel: Energy spectrum of a conduction electron in a magnetic field, *J. Exp. Theor. Phys.* **19** (1964), 634–645.

and recently confirmed by several groups observing graphene lattices in a homogeneous magnetic field.

How is this related to our problem?

We employ the trick originally proposed in

M.A. Shubin: Discrete magnetic Laplacian, *Commun. Math. Phys. 164* (1994), 259–275.

and consider a *rotation algebra* A_μ generated by elements u, v such that $uv = \mathrm{e}^{2\pi i\mu} vu$. It is simple for $\mu \notin \mathbb{Q}$, thus having *faithful representations*.

We construct two representations of A_μ which map a single element $u + v + u^{-1} + v^{-1} \in A_\mu$ to L_A and $H_{\mu,2,\theta}$, respectively, which implies that their spectra coincide, $\sigma(L_A) = \sigma(H_{\mu,2,\theta})$.

Thus we get a nontrivial result *in a cheap way*: using the duality and the fact that the function η is *locally analytic* we can complete the result from

P.E., D. Vašata: Cantor spectra of magnetic chain graphs, *J. Phys. A: Math. Theor. 50* (2017), 165201.

Theorem

(d) *If $\alpha \neq 0$ and $\mu \notin \mathbb{Q}$, then $\sigma(-\Delta_{\alpha,A})$ does not depend on θ and it is a disjoint union of the isolated-point family $\{n^2 |\, n \in \mathbb{N}\}$ and Cantor sets, one inside each interval $(-\infty, 1)$ and $\left(n^2, (n+1)^2\right)$, $n \in \mathbb{N}$. Moreover, the overall Lebesgue measure of $\sigma(-\Delta_{\alpha,A})$ is zero.*

Hausdorff dimension

The almost Mathieu operator is one of the most intensely studied, and there are other results which have implications for our magnetic chain model. Let us mention two of them with their consequences; recall that a *G_δ set* is a countable intersection of open sets.

Corollary

Let $A_j = \mu j + \theta$ for some $\mu, \theta \in \mathbb{R}$ and every $j \in \mathbb{Z}$. There exists a dense G_δ set of the slopes μ for which, and all θ, the Haussdorff dimension

$$\dim_H \sigma(-\Delta_{\alpha,A}) = 0$$

Y. Last, M. Shamis: Zero Hausdorff dimension spectrum for the almost Mathieu operator, *Commun. Math. Phys.* **348** (2016), 729–750.

Corollary

There is another dense set of the slopes μ, with positive Hausdorff measure, for which, on the contrary, $\dim_H \sigma(-\Delta_{\alpha,A}) > 0$.

B. Helffer, Qinghui Liu, Yanhui Qu , Qi Zhou: Positive Hausdorff dimensional spectrum for the critical almost Mathieu operator, *Commun. Math. Phys.* **368** (2019), 369–382.

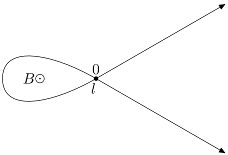
Resonance count

Presence of a magnetic field can influence also other quantum graphs properties. Recall the high-energy asymptotics of the *resonance counting function* we discussed in Lecture III, and expose such a graph Γ with leads to a field described by a vector potential A referring to it as Γ_A.

Using the technique from [Davies-E-Lipovský'10], reducing the problem to analysis of the core graph with energy-dependent boundary conditions at the 'outer' vertices, one can check the following claim:

If Γ is *Weyl*, $W = \sum_{j=1}^{N} l_j$, then Γ_A is *also Weyl*.

On the other hand: for *non-Weyl* graphs the field may change their effective size. Here is a simple example:



This (Kirchhoff) graph is non-Weyl for $A = 0$, and thus *for any A*.

Resonance count, continued

The resonance condition for such a graph is easily found to be

$$-2\cos\phi + \mathrm{e}^{-ik\ell} = 0,$$

where $\phi = A\ell$ is the magnetic flux through the loop. The senior term, $\mathrm{e}^{ik\ell}$, is missing, so by Langer theorem the effective size is $W = \frac{1}{2}\ell$ provided the *ℓ-independent term is nonzero*.

However, for $\phi = \pm\pi/2 \pmod{\pi}$, this term *disappears*. The effective size of the graph is then zero; it is straightforward to see that in the present case there are *no resonances at all*.

P.E., J. Lipovský: Non-Weyl resonance asymptotics for quantum graphs in a magnetic field, *Phys. Lett.* **A375** (2011), 805–807.

Recall that (in the used units) the *flux quantum* is 2π, hence resonances are absent for *odd multiples* of *a quarter* of the quantum. One could compare it with the ring chain where the absolutely continuous spectrum disappeared for *odd multiples* of *one half* of the quantum.

Leaky loops with a magnetic field

Magnetic field effects can also be seen in *leaky graphs*. To give an example, consider a singular interaction supported by a *planar loop* in a homogeneous field with the vector potential $A = \frac{1}{2}B(-x_2, x_1)$.

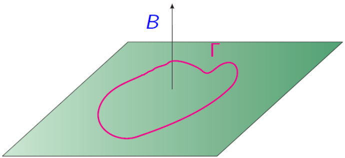
An important physical question concerns the existence of *persistent currents*, in other words, a nonzero probability flux along the loop satisfying the relation

$$\frac{\partial \lambda_n(\phi)}{\partial \phi} = -\frac{1}{c} I_n,$$

where $\lambda_n(\phi)$ is the nth eigenvalue of the Hamiltonian

$$H_{\alpha,\Gamma}(B) := (-i\nabla - A)^2 - \alpha\delta(x - \Gamma)\,;$$

here ϕ is again the magnetic flux (the quantum of which is $2\pi\frac{\hbar c}{|e|}$)



Persistent currents

We can find the strong-coupling asymptotics as we did in Lecture V using the same technique, but a different comparison operator, namely

$$S_\Gamma(B) = -\frac{\mathrm{d}^2}{\mathrm{d}s^2} - \frac{1}{4}k(s)^2$$

on $L^2(0,L)$ with $\psi(L-) = \mathrm{e}^{iB|\Omega|}\psi(0+)$ and $\psi'(L-) = \mathrm{e}^{iB|\Omega|}\psi'(0+)$, where Ω is the area encircled by Γ and $B|\Omega|$ is the *flux*.

Theorem

Let Γ be a C^4-smooth. The for large α the operator $H_{\alpha,\Gamma}(B)$ has a non-empty discrete spectrum and the jth eigenvalue behaves as

$$\lambda_j(\alpha, B) = -\frac{1}{4}\alpha^2 + \mu_j(B) + \mathcal{O}(\alpha^{-1}\ln\alpha),$$

where $\mu_j(B)$ is the jth eigenvalue of $S_\Gamma(B)$ and the error term is uniform in B. In particular, for a fixed j and α large enough the function $\lambda_j(\alpha,\cdot)$ cannot be constant giving rise to a persistent current.

P. Exner, K. Yoshitomi: Persistent currents for 2D Schrödinger operator with a strong δ-interaction on a loop, *J. Phys. A: Math. Gen.* **35** (2002), 3479–3487.

Concentric δ-shells

To give one more example, consider first a specific leaky system the Hamiltonian of which contains δ-interactions supported by *concentric shells*,

$$H_\beta = -\Delta + \beta \sum_n \delta(|x| - r_n) \quad \text{in } L^2(\mathbb{R}^\nu),\ \nu \geq 2$$

with $r_n := \left(n - \frac{1}{2}\right)s,\ d > 0,\ n = 1, 2, \dots$, and let h_β be the Hamiltonian of the corresponding 1D *Kronig-Penney model*

In the nontrivial case, $\beta \neq 0$, the spectrum is already interesting enough:

- $\sigma_{\mathrm{ess}}(H_\beta) = [E_\beta, 0)$, where $E_\beta := \inf \sigma(h_\beta)$
- it consists of *interlacing intervals* of *a.c.* and *dense p.p.* spectrum
- $\sigma_{\mathrm{disc}}(H_\beta)$ is *empty* for $\nu \geq 3$ and *infinite* for $\nu = 2$; Malcolm Brown coined the term *Welsh eigenvalues* for $\sigma_{\mathrm{disc}}(H_\alpha)$ in the latter case

P.E., M. Fraas: On the dense point and absolutely continuous spectrum for Hamiltonians with concentric δ shells, *Lett. Math. Phys.* **82** (2007), 25–37.

The same as is known to be true for *regular, radially periodic* potentials

B.M. Brown, M.S.P. Eastham , A.M. Hinz, T. Kriecherbauer, D.K.R. McCornack, K. Schmidt: Welsh eigenvalues of radially periodic Schrödinger operators, *J. Math. Anal. Appl.* **225** (1998), 347–357.

K.M. Schmidt: Critical coupling constants and eigenvalue asymptotics of perturbed periodic Sturm-Liouville operators, *Commun. Math. Phys.***211** (2000), 645–685.

Welsh eigenvalues vs. Aharonov & Bohm

Let us now insert a *singular magnetic flux* into circles center,

$$H_{\alpha,\beta} = (-i\nabla - A)^2 + \alpha \sum_n \delta(|x| - r_n)\,,$$

where the field is *zero* away from the center, corresponding to

$$A(x,y) = \frac{\phi}{2\pi}\left(-\frac{y}{r^2}, \frac{x}{r^2}\right);$$

since in the rational units the flux quantum is 2π, we introduce $\alpha := \frac{\phi}{2\pi}$.

The free Aharonov-Bohm Hamiltonian $H_{\alpha,0} := (-i\nabla - A)^2$ is defined on the *magnetic Sobolev space*. The integer part of α can be removed by a gauge transformation, hence we consider $\alpha \in (0,1)$ only.

The radial symmetry allows us to use the partial wave decomposition. As usual we introduce $U : L^2(\mathbb{R}_+, r\mathrm{d}r) \to L^2(\mathbb{R}_+)$ acting as $Uf(r) = r^{1/2} f(r)$ to get

$$L^2(\mathbb{R}^2) = \bigoplus_{l\in\mathbb{Z}} U^{-1} L^2(\mathbb{R}_+) \otimes S_l\,,$$

Welsh eigenvalues vs. Aharonov & Bohm, contd.

$$H_{\alpha,0} = \bigoplus_{l} U^{-1} H_{\alpha,0,l} U \otimes I_l \,,$$

where I_l is the identity operator on S_l and the *radial part* is

$$H_{\alpha,0,l} := -\frac{d^2}{d^2 r} + \frac{1}{r^2} c_{\alpha,l} \,, \quad c_{\alpha,l} := -\frac{1}{4} + (l+\alpha)^2,$$

$$D(H_{\alpha,0,l}) := \{ f \in L^2(\mathbb{R}_+) \,:\, -f'' + \frac{c_{\alpha,l}}{r^2} f \in L^2(\mathbb{R}_+),$$

$$\lim_{r\to 0^+} r^{\alpha-1/2} f(r) = 0 \;\text{ if }\; l = 0,$$

$$\lim_{r\to 0^+} r^{1-\alpha-1/2} f(r) = 0 \;\text{ if }\; l = -1 \}.$$

Note that this is a ‘pure’ Aharonov-Bohm operator without *an additional singular interaction* at the origin

R. Adami, A. Teta: On the Aharonov-Bohm Hamiltonian, *Lett. Math. Phys.* **43** (1998), 43–54.

L. Dąbrowski, P. Šťovíček: Aharonov-Bohm effect with δ type interaction, *J. Math. Phys.* **39** (1998), 47–72.

Welsh eigenvalues vs. Aharonov & Bohm, contd.

Now we add the *δ-interactions* at the points $r = r_n$, $n = 1, 2, \dots$, and find easily the following elementary properties of $H_{\alpha,\beta}$:

Proposition

Suppose that $\beta \neq 0$, then

- $\sharp\sigma_{\rm disc}(H_{0;\beta}) = \infty$
- $\sigma_{\rm disc}(H_{\frac12;\beta}) = \emptyset$
- $\sigma_{\rm disc}(H_{\alpha,\beta}) = \sigma_{\rm disc}(H_{1-\alpha,\beta})$
- *if $\sigma_{\rm disc}(H_{\alpha,\beta}) \neq \emptyset$, then eigenvalues of $H_{\alpha,\beta}$ are nondecreasing in the interval $[0, \frac12]$ and $\lambda_j(\alpha') \geq \lambda_j(\alpha)$ holds for a fixed j if $\alpha' \geq \alpha$*

The question is now: How $\sigma_{\rm disc}(H_{\alpha,\beta})$ looks like for $\alpha \in (0, \frac12)$?

To this aim one can use *oscillation theory tools* adapting the results of the paper [Schmidt'00, loc.cit.] to our singular interactions.

Welsh eigenvalues vs. Aharonov & Bohm, contd.

The discrete spectrum comes from the partial wave component $H_{\alpha,\beta,0}$ being determined by $c_{\alpha,0} = \alpha^2 - \frac{1}{4}$.

Let u be the d-periodic real-valued solution of the *1D comparison problem*,

$$h_\beta u = E_\beta u,$$

corresponding to the threshold E_β. Then we make the following claim:

Theorem

Suppose that $\alpha \in (0, \frac{1}{2})$ and put

$$c_{\mathrm{crit}} := -\frac{1}{4} \left(\frac{1}{d} \int_0^d \frac{1}{u^2} \, \mathrm{d}x \right)^{-1} \left(\frac{1}{d} \int_0^d u^2 \, \mathrm{d}x \right)^{-1},$$

then E_β is an accumulation point of $\sigma_{\mathrm{disc}}(H_{\alpha,\beta,0})$ provided $\frac{c_{\alpha,0}}{c_{\mathrm{crit}}} > 1$, while for $\frac{c_{\alpha,0}}{c_{\mathrm{crit}}} \le 1$ the operator has at most finite number of eigenvalues below E_β with the multiplicity taken into account.

P.E., S. Kondej: : Aharonov and Bohm versus Welsh eigenvalues, *Lett. Math. Phys. 108* (2018), 2153–2167.

Welsh eigenvalues vs. Aharonov & Bohm, contd.

Note that in case of regular potentials the number c_{crit} is sometimes called *Knesser constant* in the literature.

Since $c_{\mathrm{crit}} > -\frac{1}{4}$ by Schwartz inequality, we get

Corollary

There exists an $\alpha_{\mathrm{crit}}(\beta) = \alpha_{\mathrm{crit}} \in (0, \frac{1}{2})$ such that for $\alpha \in (0, \alpha_{\mathrm{crit}})$ the operator $H_{\alpha,\beta}$ has infinitely many eigenvalues accumulating at the threshold E_0, the multiplicity taken into account, while for $\alpha \in [\alpha_{\mathrm{crit}}, \frac{1}{2})$ the cardinality of the discrete spectrum is finite.

Moreover, since in our case u is known (quasi)explicitly, we find easily that $\alpha_{\mathrm{crit}}(\beta) = \mathcal{O}(\beta^2)$ holds as $\beta \to 0$ and

$$\alpha_{\mathrm{crit}}(\beta) = \frac{1}{2} + \mathcal{O}(\beta^2 \mathrm{e}^{-|\beta| d/2}) \quad \text{as} \quad \beta \to -\infty\,,$$

$$\alpha_{\mathrm{crit}}(\beta) = \frac{1}{2} + \mathcal{O}(\beta^{-1}) \quad \text{as} \quad \beta \to \infty\,;$$

note that the *sign of β* shows up only in the error term.

Emptiness of $\sigma_{\rm disc}(H_{\alpha,\beta})$ for weak interactions

The next claim comes from properties of the quadratic form of the operator $H_{\alpha,\beta,0} - E_\beta$. Any $f \in D(H_{\alpha,\beta,0})$ can be written as $u\chi$ with $\chi \in H_0^{2,2}(\mathbb{R}_+)$, and

$$q_{\alpha;\beta,0}[u\chi] = -\int_0^\infty u\chi(u\chi)''\,\mathrm{d}r + c_{\alpha,0}\int_0^\infty u^2\frac{\chi^2}{r^2}\,\mathrm{d}r - E_\beta\|u\chi\|^2$$

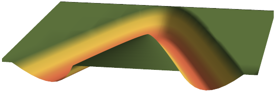
Examining the right-hand side, one can prove that the form is *non-negative for small enough* $|\beta|$, and consequently, referring again to the paper [E-Kondej'18, loc.cit.], we have

Theorem

Given $\alpha \in (0, \frac{1}{2})$, there exists a $\beta_0 > 0$ such that for any $|\beta| < \beta_0$ the operator $H_{\alpha;\beta}$ has empty discrete spectrum.

Soft quantum waveguides

Let us turn to the second topic mentioned in the opening. The leaky wire model with its *zero width* is also an idealization; to get something more realistic we replace the δ function by a finite *potential well*



For simplicity we will work in the simplest two-dimensional setting. To begin with, let us collect the hypotheses we will use:

Let $\Gamma: \mathbb{R} \to \mathbb{R}^2$ be an infinite and smooth planar curve without self-intersections, parametrized by its arc length s. We introduce again the signed curvature $\gamma: \gamma(s) = (\dot\Gamma_2\ddot\Gamma_1 - \dot\Gamma_1\ddot\Gamma_2)(s)$ and assume that

- (a) Γ is *C^2-smooth* so, in particular, $\gamma(s)$ makes sense,
- (b) γ is either of *compact support*, $\operatorname{supp}\gamma \subset [-s_0, s_0]$ for some $s_0 > 0$, or Γ is *C^4-smooth* and $\gamma(s)$ together with its first and second derivatives tend to zero as $|s| \to \infty$,
- (c) $|\Gamma(s) - \Gamma(s')| \to \infty$ holds as $|s - s'| \to \infty$ (no U-shapes, etc.).

The interaction support

Recall that one can *reconstruct the curve* from the knowledge of γ, up to Euclidean transformations: putting $\beta(s_2, s_1) := \int_{s_1}^{s_2} \gamma(s)\,\mathrm{d}s$, we have

$$\Gamma(s) = \left(x_1 + \int_{s_0}^{s} \cos\beta(s_1, s_0)\,\mathrm{d}s_1,\, x_2 - \int_{s_0}^{s} \sin\beta(s_1, s_0)\,\mathrm{d}s_1\right)$$

for some $s_0 \in \mathbb{R}$ and $x = (x_1, x_2) \in \mathbb{R}^2$. Next we define the strip Ω^a by

$$\Omega^a := \{x \in \mathbb{R}^2 :\ \mathrm{dist}(x, \Gamma) < a\},$$

in particular, $\Omega_0^a := \mathbb{R} \times (-a, a)$ corresponds to a straight line for which we use the symbol Γ_0. We assume that

- (d) Ω^a *does not intersect itself*, in particular, $a\|\gamma\|_\infty < 1$ holds for the strip halfwidth of Γ

which ensures that the points of Ω^a can be uniquely parametrized as follows,

$$x(s, u) = \left(\Gamma_1(s) - u\dot{\Gamma}_2(s), \Gamma_2(s) + u\dot{\Gamma}_1(s)\right),$$

where $N(s) = (-\dot{\Gamma}_2(s), \dot{\Gamma}_1(s))$ is the *unit normal vector* to Γ at the point s.

The potential 'ditch'

We will deal with Schrödinger operators having an *attractive potential* supported in Ω^a. To this aim, we consider

- a nonnegative $V \in L^\infty(\mathbb{R})$ with $\mathrm{supp}\, V \subset [-a, a]$

(where $V \geq 0$ is assumed for convenience only) and to define

$$\tilde{V} :\ \Omega^a \to \mathbb{R}_+,\ \ \tilde{V}(x(s,u)) = V(u),\ \text{ and }\ H_{\Gamma,V} = -\Delta - \tilde{V}(x);$$

in view of assumption (e) the operator domain is $D(-\Delta) = H^2(\mathbb{R}^2)$

It is also useful to introduce the *channel-profile* operator on $L^2(\mathbb{R})$,

$$h_V = -\partial_x^2 - V(x)$$

with the domain $H^2(\mathbb{R})$ which has in accordance with (e) a nonempty and finite discrete spectrum such that

$$\epsilon_0 := \inf \sigma_{\rm disc}(h_V) = \inf \sigma(h_V) \in \big(-\|V\|_\infty, 0\big),$$

where the ground-state eigenvalue ϵ_0 is *simple* and the associated eigenfunction $\phi_0 \in H^2(\mathbb{R})$ can be chosen *strictly positive*.

Spectrum of $H_{\Gamma,V}$

If the strip axis Γ is straight, the spectrum is easily found using separation of variables; it is $\sigma(H_{\Gamma_0,V}) = \sigma_{\mathrm{ess}}(H_{\Gamma_0,V}) = [\epsilon_0, \infty)$.

On the other hand, if the ditch is curved but *straight outside* a compact, or at least *asymptotically straight* in the sense of (b), one can use Weyl's criterion to prove the essential spectrum is preserved:

Proposition

Under assumptions (a)–(e) *we have* $\sigma_{\mathrm{ess}}(H_{\Gamma,V}) = [\epsilon_0, \infty)$

As is the case of hard-wall waveguides or leaky wires, the question is whether the curvature would give rise to *bound states*.

It is not clear at this moment whether there is a universal existence result similar to those we were able to demonstrate in the indicated cases, but we have at least some partial answers:

- *asymptotic results* based on our previous knowledge
- a *quantitative criterion* based on Birman-Schwinger principle

Asymptotic results

We know from Lecture IV that $-\Delta - \alpha\delta(x-\Gamma)$ can be approximated in the *norm-resolvent sense* by Schrödinger operators with potentials *transversally scaled*, V_ε : $V_\varepsilon(u) = \frac{1}{\varepsilon} V\left(\frac{u}{\varepsilon}\right)$. This allows us to prove:

Proposition

Consider a non-straight C^2-smooth curve $\Gamma : \mathbb{R} \to \mathbb{R}^2$ such that $|\Gamma(s) - \Gamma(s')| > c|s - s'|$ holds for some $c \in (0,1)$. If the support of its signed curvature γ is noncompact, assume, in addition to (b), that $\gamma(s) = \mathcal{O}(|s|^{-\beta})$ with some $\beta > \frac{5}{4}$ as $|s| \to \infty$. Then $\sigma_{\rm disc}(H_{\Gamma,V_\varepsilon}) \neq \emptyset$ holds for all ε small enough.

Consider, on the other hand, a *flat-bottom* waveguide, $V_{J,0}(u) = V_0\chi_J(u)$, where χ_J refers to an interval $J \subset [-a_0, a_0]$. Using the *high potential wall* limit and the existence result from Lecture I we can conclude:

Proposition

Let Γ be non-straight and assume that assumptions (a)–(d) are satisfied, then $\sigma_{\rm disc}(H_{\Gamma,V_\varepsilon}) \neq \emptyset$ holds for all V_0 large enough.

A quantitative criterion

We have met Birman-Schwinger principle, standard and generalized, in Lecture IV. Since the potential is supported in Ω^a only, we may apply it,

- use the *curvilinear* (Fermi, parallel) coordinates in Ω^a,
- *'straighten'* the strip and treat $H_{\Gamma,V}$ as a *perturbation* of $H_{\Gamma_0,V}$

Theorem

Let assumptions (a)–(e) be valid and set

$$\mathcal{C}^{\kappa}_{\Gamma,V}(s,u;s',u') = \frac{1}{2\pi}\,\phi_0(u)V(u)\left[(1+u\gamma(s))^{1/2}\,K_0(\kappa|x(s,u)-x(s',u')|)\,(1+u'\gamma(s'))^{1/2}\right.$$
$$\left. -K_0(\kappa|x_0(s,u)-x_0(s',u')|)\,\right]\,V(u')\phi_0(u')$$

for all (s,u), $(s',u') \in \Omega^a_0$, *then we have* $\sigma_{\rm disc}(H_{\Gamma,V}) \neq \emptyset$ *provided*

$$\int_{\mathbb{R}^2} \mathrm{d}s\mathrm{d}s' \int_{-a}^{a}\int_{-a}^{a} \mathrm{d}u\mathrm{d}u'\,\mathcal{C}^{\kappa_0}_{\Gamma,V}(s,u;s',u') > 0$$

holds for $\kappa_0 = \sqrt{-\epsilon_0}$.

P.E.: Spectral properties of soft quantum waveguides, *J. Phys. A: Math. Theor.* **53** (2020), 355302.

One more existence result

The integral kernel in the criterion involves the Euclidean distances between points of the curved strip:

$$|x(s,u)-x(s',u')|^2 = |\Gamma(s)-\Gamma(s')|^2 + u^2 + u'^2 - 2uu'\cos\beta(s,s') + 2(u\cos\beta(s,s')-u')\int_{s'}^{s}\sin\beta(\xi,s')\,\mathrm{d}\xi,$$

where the first term on the right-hand side of this formula, expressing Euclidean distance of points on the strip 'axis', satisfies

$$|\Gamma(s)-\Gamma(s')|^2 = \int_{s'}^{s}\int_{s'}^{s}\cos\beta(\xi,\xi')\,\mathrm{d}\xi\,\mathrm{d}\xi' < |\Gamma_0(s)-\Gamma_0(s')|^2 = |s-s'|^2$$

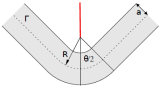
whenever *the bend is nontrivial*. This property was decisive in the leaky wire case; using it we get from the above theorem the following claim:

Corollary

Let $\mathcal{V}_{\epsilon_0}$ be the family of potentials V satisfying assumptions (d), (e), and $\inf\sigma(h_V)=\epsilon_0$. *Then to any $\epsilon_0>0$ there exists an $a_0=a_0(\epsilon_0)$ such that* $\sigma_{\rm disc}(H_{\Gamma,V})\neq\emptyset$ *holds for all $V\in\mathcal{V}_{\epsilon_0}$ with* $\mathrm{supp}\,V\subset[-a_0,a_0]$.

Remarks

- Birman-Schwinger principle is not the only tool available; a natural alternative is to employ a *variational method*. In this way the bound state existence was proved for *bookcover-shaped* potential ditches



Source: the cited paper

S. Kondej, D. Krejčiřík, J. Kříž: Soft quantum waveguides with a explicit cut locus, arXiv:2007.10946

- It is a particular example, but the bound state existence was proved there for *arbitrarily shallow channels*; the question arises whether the same could be true in other situations.
- Moreover, these results open a plethora of questions about *soft waveguide* properties in different dimensions, different geometries, topological properties of such *potential ditch networks*, etc.
- To quote a fresh result, if you have a family of *soft quantum loops* of a fixed length $|\Gamma|$ and profile V, the *ground state* of the operator $H_{\Gamma,V}$ is *maximized by a circular shape*.

P.E., V. Lotoreichik: Optimization of the lowest eigenvalue of a soft quantum ring, *Lett. Math. Phys.* **111** (2021), 28.

This is not the end, of course

If you tend to feel that these lectures have fully exhausted, fully or almost fully, the title of this minicourse, better think twice. There is a number of equally interesting problems to be treated, for instance

- *Inverse problems:* to what extent we can reconstruct geometry of a waveguide or a network from its spectral and scattering data? We have seen, for instance, that in the limiting case when the effective Hamiltonian is $-\frac{\mathrm{d}^2}{\mathrm{d}s^2} - \frac{1}{4}k(s)^2$ there is a *sign ambiguity*; the question is whether it could be removed for finite guide width or well depth.
- *Absence of positive lower bound* for graph edge lengths makes the spectral analysis much more involved. Note that often we encounter *fractal structures* for which such models could be useful.

  P.E., A. Kostenko, M. Malamud, H. Neidhardt: Spectral theory of infinite quantum graphs, *Ann. H. Poincaré* **19** (2018), 3457–3510.
- Putting aside traditional *electromagnetic waveguides* there are other interesting examples of guided dynamics. One recently popular relies on *Dirac equation* (think of graphene ribbons!), other examples are provided by the *wave equation*, *elasticity*, etc.

This is not the end, of course

- The problems we discussed here had mostly *one-body character*, many-body analysis of waveguides and graphs is much less developed. As in the atomic physics, a natural intermediary step is represented by *nonlinear* one-body problems.

D. Noja: Nonlinear Schrödinger equation on graphs: recent results and open problems, *Phil. Trans. Roy. Soc.* **A372** (2014), 20130002.

- Quantum graphs with *random parameters* offer the opportunity to study the effects of *localization* and *delocalization* in this context.

F. Klopp, K. Pankrashkin: Localization on quantum graphs with random vertex couplings, *J. Stat. Phys.* **131** (2008), 651–673.

M. Aizenman, R. Sims, S. Warzel: Absolutely continuous spectra of quantum tree graphs with weak disorder, *Commun. Math. Phys.* **264** (2006), 371–389.

- Quantum graphs are natural laboratory to study *quantum chaos* and *ergodic properties* of such dynamics.

T. Kottos, U. Smilansky: Quantum chaos on graphs, *Phys. Rev. Lett.* **79** (1997), 4794–4797.

S. Gnutzmann, J.P. Keating, F. Piotet: Eigenfunction statistics on quantum graphs, *Ann. Phys.* **25** (2010), 2595–2640.

- And this, again, is by far not all.

Instead of a summary

Maybe the best moral to draw from this minicourse is that quantum physics, in particular, that of waveguides, graphs, and networks is still full of *challenges* and to mention, as a parting gift to you, a few of them.

Claims with the potential to make your night sleepless are of two sorts. With some of them you have no doubt they are right, but they defy efforts to be proven. Mathematics offers famous examples such as *Fermat's last theorem* (proved by Andrew Wiles after 356 years) or the equally celebrated *Riemann conjecture* (open since 1859),

or several others for which the Clay Institute is ready to make you a rich man (or lady). But this may not be their most attractive feature – recall *Grigory Perelman* who famously said: "Do you really need million dollars when you proved Poincaré conjecture?"

Quantum theory is not that old but it also has, or had, its longstanding open questions of this type, some resolved, some still open.

Instead of a summary

As examples one can mention the *Bethe-Sommerfeld conjecture* that appeared in Lecture III: it was stated 1933, the first rigorous result is due to M. Skriganov in 1987, a rather general one due to L. Parnovski in 2008,

or the *Ten Martini Problem* arising for the work of M. Azbel in 1964 and D. Hofstadter in 1976, resolved by A. Avila and S. Jitomirskaya in 2009,

as well as other, sometimes still open questions for which we can refer to

B. Simon: Schrödinger operators in the twenty-first century, in *Mathematical Physics 2000*, Imperial College London; pp. 283–288.

Let us mention one such open problem in the area we have discussed here concerning the *absolute continuity* of the spectrum of *periodic waveguides*.

Let $-\Delta_{\mathrm{D}}^{\Omega}$ refer to a *periodically curved tube* in $\mathbb{R}^d$, $d = 2, 3$. One expects that $\sigma(-\Delta_{\mathrm{D}}^{\Omega})$ is *purely a.c.* but for $d = 3$ we only know that to any $E > 0$ there is $a_E > 0$ such that the claim holds in $[0, a^{-2}\kappa_1^2 + E]$ for *all tube radii* $a < a_E$. A similar question for $d = 2, 3$ concerns *periodic leaky wires*.

F. Bentosela, P. Duclos, P. Exner: Absolute continuity in periodic thin tubes and strongly coupled leaky wires, *Lett. Math. Phys.* **65** (2003), 75–82.

A. Sobolev, J. Walthoe: Absolute continuity in periodic waveguides, *Proc. London Math. Soc.* **85** (2002), 717–741.

Instead of a summary

However, in other open problems *we do not know the answer*, for instance

- The *Bethe-Sommerfeld conjecture* again, now in waveguides. We know that for $-\Delta_D^{\Omega_0} + V$ in a *straight strip* with a *bounded* and *periodic* perturbation V only a *finite number of gaps* is open if

$$\frac{\text{period}}{\text{width}} \lesssim 0.20242$$

D.I. Borisov: Bethe-Sommerfeld conjecture for periodic Schrödinger operators in strip, *J. Math.Anal.Appl.* **479** (2019), 260–282.

- On the other hand, there are 'exotic' examples where such a claim is *not* valid, thus the question arises: Under *which conditions* periodic waveguides have the *BS property*?

- We have solved the *ground shape optimization* problem for loop-shaped waweguides or leaky wires assuming their *trivial* topology. What would be the answer if such a loop is a *trefoil* or a more complicated knot?

Instead of a summary

- We know that a bent waveguide or a leaky wire has a *nonempty discrete spectrum*. Let us expose it to a *homogeneous magnetic field*. If will change both the eigenvalues and the essential spectrum, however, by a continuity argument, for a *weak* field the discrete spectrum is still there. One asks: Will it survive a *strong* field?
- Or one more seemingly simple problem, the *Wannier-Stark δ-interaction system*, that is, the one with the Hamiltonian

$$-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \alpha \sum_{n\in\mathbb{Z}} \delta(x - na) - Fx$$

  on $L^2(\mathbb{R})$ with some nonzero α and F and an $a > 0$. If the periodic Kroning-Penney potential is replaced by a *regular* one, the spectrum is *absolutely continuous*, for a *strongly singular one* such as δ' it is *pure point*, dense or not depending on the properties of F.
- A transition from pure point spectrum for *small* $|F|$ to *continuous* one for strong field was conjectured, but reality may be more complicated

R.L. Frank, S. Larson: On the spectrum of the Kronig-Penney model in a constant electric field, arXiv:2104.10256

- And this list could continue for a long time ...

However, I think time came to say

Thank you for your attention!