Singular Schrödinger operators and Robin billiards: geometry, spectra and asymptotic expansions

Pavel Exner

Doppler Institute
for Mathematical Physics and Applied Mathematics
Prague

in collaboration with *Jussi Behrndt*, *Jaroslav Dittrich*, *Michal Jex*, *Sylwia Kondej*, *Christian Kühn*, *Vladimir Lotoreichik*, and *Konstantin Pankrashkin*

A talk at the conference Operators, Operator Families and Asymptotics

University of Bath, May 16, 2016

Leaky quantum graphs and their generalizations

The first main object of interest in this talk are singular Schrödinger operators that can formally written as

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

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

Motivation: (a) Interesting mathematical objects, in particular, since their spectral properties reflect the geometry of Γ
(b) an alternative model of *quantum graphs* and *generalized graphs* with the advantage that tunneling between edges is not neglected

Here we shall consider the simplest situation where Γ is a *smooth manifold* in $\mathbb{R}^n$ having in mind 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

The talk outline

We will be concerned with the *discrete spectra* of such operators, in particular, with *asymptotic expansions* of the eigenvalues with respect to the parameters of the model.

- Setting the scene: definition of the operators
- Discrete spectrum induced by the singular interaction
- Strong coupling eigenvalue asymptotics
  - Closed manifolds
  - Curves with ends
  - Surfaces with a boundary
  - δ' interactions
- A digression: Robin billiard counterparts
- A geometric perturbation asymptotics
- Asymptotic distribution of eigenvalues
- Some open questions

Definition of the Hamiltonian

The easiest way to introduce a δ-interaction in the case $\operatorname{codim}\Gamma = 1$ is to employ the quadratic form,

$$\psi \mapsto \|\nabla\psi\|^2_{L^2(\mathbb{R}^d)} - \alpha\int_\Gamma |\psi(x)|^2 \mathrm{d}x\,,$$

which is closed and below bounded in $W^{1,2}(\mathbb{R}^d)$, $d = 2,3$; the second term makes sense in view of the standard Sobolev embedding.

For *smooth manifolds* we can use an alternative definition by boundary conditions: $H_{\alpha,\Gamma}$ acts as $-\Delta$ on functions from $W^{2,2}_{\mathrm{loc}}(\mathbb{R}^d \setminus \Gamma)$, which are continuous and exhibit a normal-derivative jump,

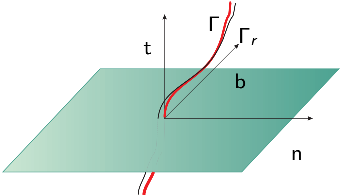
$$\frac{\partial\psi}{\partial n}(x)\Big|_+ - \frac{\partial\psi}{\partial n}(x)\Big|_- = -\alpha\psi(x)$$

Moreover, for $\operatorname{codim}\Gamma = 1$ one can consider other, more singular interactions. The prime example is a *δ'-interaction* supported by Γ in which the roles of ψ and $\frac{\partial\psi}{\partial n}$ are switched; more about that a bit later.

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

This is more complicated but one can use again boundary conditions, appropriately modified. Furthermore, for an infinite curve Γ corresponding 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



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

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

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

$$\begin{aligned} \Xi(f)(s) &:= -\lim_{r\to 0} \frac{1}{\ln r} f\restriction_{\Gamma_r}(s)\,, \\ \Omega(f)(s) &:= \lim_{r\to 0} \left[f\restriction_{\Gamma_r}(s) + \Xi(f)(s) \ln r \right]\,, \end{aligned}$$

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

Then the 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 $\alpha = \infty$!

Spectrum of $H_{\alpha,\Gamma}$

Consider first the δ-interaction with a *finite* support, $|\Gamma| < \infty$.

In this case it is easy to check that $\sigma_{\mathrm{ess}}(H_{\alpha,\Gamma}) = \mathbb{R}_+$ holds.

On the other hand, the existence of a negative discrete spectrum is *dimension dependent*. For $d = 2$ bound states exist whenever $|\Gamma| > 0$, in particular, we have a weak-coupling expansion [Kondej-Lotoreichik'14]

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

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 by [Antoine-Gesztesy-Shabani'87] we have

$$\sigma_{\mathrm{disc}}(H_{\alpha,\Gamma}) \neq \emptyset \quad \text{iff} \quad \alpha R > 1$$

Critical coupling for $\operatorname{codim}\Gamma = 2$

The interaction is more singular but still it behaves with respect to weak coupling as a regular potential in three dimensions:

Theorem (E-Kondej'08)

For a fixed $\alpha \in \mathbb{R}$ there exists a $L_\alpha > 0$ such that the $H_{\alpha,\Gamma}$ has no discrete spectrum for $|\Gamma| < L_\alpha$. On the other hand, if $|\Gamma| > 2\pi\,\mathrm{e}^{2\pi\alpha-\psi(1)}$, then there is at least one bound state.

The existence is easy, one has to consider a straight Γ and use Dirichlet bracketing. The nonexistence is a bit more involved and requires to estimate the norm of the generalized Birman-Schwinger operator.

The δ' interaction in the plane

This case is more involved because the answer depends on the *topology* of Γ. In particular, it is easy to see that the corresponding Hamiltonian $H_{\beta,\Gamma}$ has always a discrete spectrum if Γ *is a loop*.

On the other hand, consider nonclosed *monotone* curves, piecewise C^1, i.e. those one can parametrize by a piecewise C^1 map $\varphi : (0, R) \to \mathbb{R}$ as

$$\Gamma = \left\{x_0 + r(\cos\varphi(r), \sin\varphi(r)) :\; r \in (0, R)\right\}$$

Theorem (Jex-Lotoreichik'16)

We have $\sigma(H_{\beta,\Gamma}) \subset \mathbb{R}_+$ *if* $\beta > 2\pi r\sqrt{1 + (r\varphi'(r))^2}$ *holds for all* $r \in (0, R)$.

Recall that *large β means weak coupling* for the δ' interaction. The proof is based on a minimax estimate and the claim extends to a wider class of curves obtained form the above on by *linear fractional transformations*.

Question: Is $\sigma(H_{\beta,\Gamma}) \subset \mathbb{R}_+$ for *any* non-closed Γ and β large enough? According to Monique Dauge, the answer seems to be *positive*.

δ interaction supported by infinite curves

A geometrically induced spectrum may exist even if Γ is infinite and $\inf \sigma_{\mathrm{ess}}(H_{\alpha,\Gamma}) < 0$. As an example, consider a *non-straight, piecewise C^1-smooth curve* $\Gamma : \mathbb{R} \to \mathbb{R}^2$ parameterized by its arc length, assuming

- $|\Gamma(s) - \Gamma(s')| \geq c|s - s'|$ 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

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

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

Theorem (E-Ichinose'01)

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

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 analogous result holds for *curves in* $\mathbb{R}^3$, under slightly stronger regularity hypotheses, with $-\frac{1}{4}\alpha^2$ replaced by the corresponding 2D point-interaction eigenvalue
- For *curved surfaces* $\Gamma \subset \mathbb{R}^3$ such a result is proved at present in the strong coupling asymptotic regime only
- *Implications for graphs:* let $\tilde{\Gamma} \supset \Gamma$ in the set sense, then $H_{\alpha,\tilde{\Gamma}} \le H_{\alpha,\Gamma}$. If the essential spectrum threshold is the same for both graphs – which is often easy to establish – and Γ fits the above assumptions, we have $\sigma_{\mathrm{disc}}(H_{\alpha,\Gamma}) \ne \emptyset$ by the minimax principle

Strong δ interaction asymptotics

If the *attraction is strong* the motion is strongly localized transversally and the geometry of Γ is manifested. Again, we exclude self-intersections.

Consider a a C^4 smooth *curve in $\mathbb{R}^2$ without ends*, either infinite or a closed loop. In the limit $\alpha \to \infty$ the j-th eigenvalue of $H_{\alpha,\Gamma}$ behaves as

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

where μ_j is the j-th eigenvalue of

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

on $L^2((0,|\Gamma|))$ for $\dim \Gamma = 1$, where κ is *curvature* of Γ.

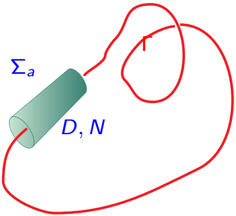
Under similar hypotheses on *smoothness* and *absence of boundaries*, the claim extends to higher dimensions, specifically

- for a curve in $\mathbb{R}^2$ we replace $-\frac{\alpha^2}{4}$ by $\epsilon_\alpha = -4\,\mathrm{e}^{2(-2\pi\alpha+\psi(1))}$
- for a surfaces in $\mathbb{R}^3$ we replace the above S by $S_\Gamma = -\Delta_\Gamma + K - M^2$, where $-\Delta_\Gamma$ is Laplace-Beltrami operator on Γ and K, M, respectively, are the corresponding *Gauss* and *mean* curvatures

Strong δ interactions, continued

There are various extensions of these results including, in particular, asymptotic expansions for *periodic manifolds*, connected or disconnected, or *loops pierced by a magnetic flux* – cf. [Ex'08] for a review

How these expansions are demonstrated: the argument has three essential ingredients. The first is *Dirichlet-Neumann bracketing* at a boundary Σ_a of a tubular neighbourhood of Γ of radius a, here sketched for a loop in $\mathbb{R}^3$



We have to care about the tube part only because the Dirichlet/Neumann Laplacian in the remaining part of $\mathbb{R}^d$ is positive

Strong δ interactions, continued

The second step we use inside the tube natural curvilinear coordinates, sometimes named *Fermi* and estimate the coefficients to squeeze the operator between those with *separated variables*. For a curve in $\mathbb{R}^2$, e.g., they are

$$\tilde{H}^{\pm}_{a,\alpha} = U^{\pm}_a \otimes 1 + 1 \otimes T^{\pm}_{a,\alpha}\,,$$

where

$$U^{\pm}_a = -(1 \mp a\|\kappa\|_\infty)^{-2} \frac{\mathrm{d}^2}{\mathrm{d}s^2} + V_\pm(s)$$

with PBC in the case of a loop, where $V_-(s) \le \frac{1}{4}\kappa^2(s) \le V_+(s)$ with an $\mathcal{O}(a)$ error. In other words, the $U^{\pm}_a$ are *$\mathcal{O}(a)$ close to S_Γ*.

The transverse operators are associated with the forms

$$t^{+}_{a,\alpha}[f] = \int_{-a}^{a} |f'(u)|^2\,\mathrm{d}u - \alpha |f(0)|^2$$

and $t^{-}_{a,\alpha}[f] = t^{-}_{a,\alpha}[f] - \|k\|_\infty(|f(a)|^2 + |f(-a)|^2)$ defined on $W^{1,2}_0(-a,a)$ and $W^{1,2}(-a,a)$, respectively.

Strong δ interactions, continued

Next we observe that for large α the presence of the boundaries causes just an exponentially small error:

Lemma

There is a positive c_N such that $T^{\pm}_{\alpha,a}$ has for α large enough a single negative eigenvalue $\kappa^{\pm}_{\alpha,a}$ satisfying

$$-\frac{\alpha^2}{4}\left(1+c_N\,\mathrm{e}^{-\alpha a/2}\right) < \kappa^{-}_{\alpha,a} < -\frac{\alpha^2}{4} < \kappa^{+}_{\alpha,a} < -\frac{\alpha^2}{4}\left(1-8\,\mathrm{e}^{-\alpha a/2}\right)$$

I the final step relate the tube radius with the coupling constant choosing $a = 6\alpha^{-1}\ln\alpha$ which yields the result

In the other dimension/codimension cases the argument is analogous. If $\operatorname{codim}\Gamma = 2$ the transverse operator describes the Dirichlet/Neumann disc of radius r with the point interaction in the centre; the error is again exponentially small as $\alpha \to -\infty$.

Curves with ends

We have seen that the described method yields for *finite* or *semifinite* curves gives the asymptotics for the number of bound states, but fails to do that for individual eigenvalues — the difference between Dirichlet and Neumann conditions imposed on the comparison operator is too big.

One conjectures that the 'correct' boundary conditions are *Dirichlet*. For a finite planar curve we can prove it:

Theorem (E-Pankrashkin'14)

Suppose γ is a C^4 smooth open arc in $\mathbb{R}^2$ of length L with regular ends; then the strong-coupling limit of the j-th negative eigenvalue of $H_{\alpha,\Gamma}$ is

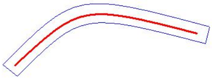
$$\lambda_j(\alpha) = -\frac{1}{4}\alpha^2 + \mu_j + \mathcal{O}\Big(\frac{\ln\alpha}{\alpha}\Big) \quad \text{as} \quad \alpha\to+\infty$$

where μ_j is the j-th eigenvalue of the operator $-\frac{\mathrm{d}^2}{\mathrm{d}s^2} - \frac{1}{4}\kappa(s)^2$ on $L^2(0,L)$ with Dirichlet b.c., where $\kappa(s)$ is as before the signed curvature of Γ at the point $s\in(0,L)$.

Curves with ends, continued

The proof starts again from bracketing estimates but no it has to be modified. The upper (Dirichlet) bound works as before, while for the lower (Neumann) we use the fact that Γ has by assumption *regular ends*, i.e. can be extended smoothly in the vicinity of the endpoints.

This allows us to take an *'extended' tubular neighbourhood*, at each endpoint longer by $a := \frac{6}{\alpha} \ln \alpha$. Now we loose the advantage of variable separation and the task is to show that the Neumann condition imposed at this distance from the curve end will have an effect which can be included into the error term.



An extended neighbourhood

Curves with ends, continued

The way to find such an estimate is to employ again the (generalized) Birman-Schwinger principle.

It says, in particular, that the eigenfunction of $H_{\alpha,\Gamma}$ corresponding to an eigenvalue $\lambda_j = -\kappa_j^2$ can be written – see, e.g. [Posilicano'04] – as

$$\psi_j(x) = \frac{1}{2\pi} \int_\Gamma K_0(\kappa_j |x - \Gamma(s)|)\, f_j(s)\, \mathrm{d}s\,,$$

where f_j is the corresponding eigenfunction of the Birman-Schwinger operator acting on $L^2(\Gamma, \mathrm{d}s)$.

The claim of the theorem then follows from simple geometric estimates combined with the exponential decay of the Macdonald function K_0 at large distances. $\square$

Curves with ends, $\operatorname{codim}\Gamma = 2$

A similar result can be obtained for a curve arc in $\mathbb{R}^3$:

Theorem (E-Kondej'16)

Let $H_{\alpha,\Gamma}$ correspond to a finite, non-closed C^4 smooth curve in $\mathbb{R}^3$ with regular ends having length L and the global Frenet frame.
(i) The cardinality of the discrete spectrum behaves asymptotically as

$$\sharp\sigma_{\mathrm{disc}}(H_{\alpha,\Gamma}) = \frac{L}{\pi}(-\epsilon_\alpha)^{1/2}(1+\mathcal{O}(\mathrm{e}^{\pi\alpha})) \quad \text{as} \quad \alpha \to -\infty\,.$$

(ii) Furthermore, the jth eigenvalue of $H_{\alpha,\Gamma}$ has the expansion

$$\lambda_j(H_{\alpha,\Gamma}) = \epsilon_\alpha + \mu_j + \mathcal{O}(\mathrm{e}^{\pi\alpha}) \quad \text{for} \quad \alpha \to -\infty\,,$$

where μ_j corresponds to same the operator S on $L^2(0,L)$ as above.

Proof is technically slightly more demanding but it follows the same basic idea as in the previous case. $\square$

Surface with a boundary

Let $\Gamma \subset \mathbb{R}^3$ be now a C^4-smooth relatively compact orientable surface with a compact Lipschitz boundary $\partial\Gamma$. In addition, we suppose that Γ can be extended through the boundary, i.e. that there exists a larger C^4-smooth surface Γ_2 such that $\overline{\Gamma} \subset \Gamma_2$.

As in the case of surfaces without a boundary we consider the operator $S_\Gamma = -\Delta_\Gamma^D + K - M^2$, where $-\Delta_\Gamma^D$ is Laplace-Beltrami operator on Γ, now with *Dirichlet condition* at $\partial\Gamma$, and K, M, respectively, are the corresponding *Gauss* and *mean* curvatures.

We denote eigenvalues of this operator as μ_j^D, $j \in \mathbb{N}$, then we have

Theorem (Dittrich-E-Kühn-Pankrashkin'16)

Let Γ be as above, then for any fixed $j \in \mathbb{N}$ we have

$$\lambda_j(H_{\alpha,\Gamma}) = -\frac{\alpha^2}{4} + \mu_j^D + o(1) \quad \text{as} \quad \alpha \to \infty\,.$$

If, in addition, Γ has a C^2 boundary, then the remainder estimate can be replaced by $\mathcal{O}(\alpha^{-1} \ln \alpha)$.

Surface with a boundary, comments on the proof

As before, the upper bound is easy because one can take a layer neighbourhood of the surface Γ itself and impose the 'right', that is, Dirichlet conditions at its boundary. Using then an estimate with separated variables, we get the result.

The lower bound can be done in two different ways. One is to construct an explicit family of operators – cf. [Dittrich-E-Kühn-Pankrashkin'16] for details – using the projection to the lowest transverse mode and its orthogonal complement, and to employ its monotonicity to prove the convergence. This gives the result but without an explicit error term; the advantage is that it requires only the Lipshitz property for $\partial\Gamma$.

An alternative is to use the same idea as for the curves with ends based on Birman-Schwinger principle. This yields an error term, but since the boundary is not a more complicated object now, we have to require a C^2 smoothness in order to be able to perform the needed geometric estimates.

Planar curves supporting a δ' interaction

If $\operatorname{codim}\Gamma = 1$ the manifold can also support more singular interactions. One possibility is the δ'-interaction. Using the curvilinear coordinates (s, u) we can define the corresponding operator $H_{\beta,\Gamma}$ through the quadratic form

$$h_{\beta,\Gamma}[\psi] = \|\nabla\psi\|^2 - \beta^{-1}\int_\Gamma |\psi(s,0_+) - \psi(s,0_-)|^2 \,\mathrm{d}s$$

defined on functions $\psi \in H^1(\mathbb{R}^2 \setminus \Gamma)$ as $\psi(s, u)$.

Alternatively, one can use boundary conditions: the operator acts as Laplacian outside the interaction support,

$$(H_{\beta,\Gamma}\psi)(x) = -(\Delta\psi)(x)$$

for $x \in \mathbb{R}^2 \setminus \Gamma$, with the domain $\mathcal{D}(H_{\beta,\Gamma}) = \{\psi \in H^2(\mathbb{R}^2 \setminus \Gamma) \mid \partial_{n_\Gamma}\psi(x) = \partial_{-n_\Gamma}\psi(x) =: \psi'(x)|_\Gamma,\ -\beta\psi'(x)|_\Gamma = \psi(x)|_{\partial_+\Gamma} - \psi(x)|_{\partial_-\Gamma}\}$, where n_Γ is the outer normal to Γ and $\psi(x)|_{\partial_\pm\Gamma}$ are the appropriate traces.

Note that the *strong-coupling limit* in this case is $\beta \to 0+$.

Strong coupling on a δ' loop

Theorem (E-Jex'13)

Let Γ be a C^4-smooth closed curve without self-intersections. Then $\sigma_{\rm ess}(H_{\beta,\Gamma}) = [0,\infty)$ and to any $n \in \mathbb{N}$ there is a $\beta_n > 0$ such that $\#\sigma_{\rm disc}(H_{\beta,\Gamma}) \geq n$ holds for $\beta \in (0,\beta_n)$. Denoting by $\lambda_j(\beta)$ the j-th eigenvalue of $H_{\beta,\Gamma}$, counted with multiplicity, we have the expansion

$$\lambda_j(\beta) = -\frac{4}{\beta^2} + \mu_j + \mathcal{O}\big(\beta|\ln\beta|\big)\,, \quad j = 1,\dots,n\,,$$

valid as $\beta \to 0_+$, where μ_j is the j-th eigenvalue of the comparison operator S, the same as before. Moreover, for the counting function $\beta \mapsto \#\sigma_d(H_{\beta,\Gamma})$ we have

$$\sharp\sigma_{\rm disc}(H_{\beta,\Gamma}) = \frac{2L}{\pi\beta} + \mathcal{O}(|\ln\beta|) \quad \text{as } \beta \to 0_+\,.$$

A similar result holds for infinite curves, cf. [Jex'14], and for strong δ' interaction supported by surfaces *without boundary*, cf. [E-Jex'14]

A digression: Robin 'billiards'

Let Ω be an open, simply connected set in $\mathbb{R}^2$ with a closed C^4 Jordan boundary $\partial\Omega = \Gamma : [0, L] \ni s \mapsto (\Gamma_1, \Gamma_2) \in \mathbb{R}^2$, with $\gamma : [0, L] \to \mathbb{R}$ being the signed curvature of Γ. We consider the boundary-value problem

$$-\Delta f = \lambda f \ \text{ in}\,\Omega\,, \quad \frac{\partial f}{\partial n} = \beta f \ \text{ on}\,\Gamma\,,$$

with $\beta > 0$, where $\frac{\partial}{\partial n}$ is the outward normal derivative.

The corresponding self-adjoint operator H_β is associated with the quadratic form

$$q_\beta[f] = \|\nabla f\|^2_{L^2(\Omega)} - \beta \int_\Gamma |f(x)|^2 \mathrm{d}s$$

defined on $\mathrm{Dom}(q_\beta) = H^1(\Omega)$.

As before we consider $S = -\frac{\mathrm{d}^2}{\mathrm{d}s^2} - \frac{1}{4}\gamma^2(s)$ on $L^2(0, L)$ with periodic b.c., and furthermore, we denote $\gamma^* = \max_{[0,L]} \gamma(s)$ and $\gamma_* = \min_{[0,L]} \gamma(s)$.

A large parameter asymptotics

Since the Robin problem can be regarded as a 'one-sided version' of our singular Schrödinger operators, one can try to employ the same technique. Its naive use, however, yields only a much weaker result,

$$-\Big(\beta + \frac{\gamma^*}{2}\Big)^2 + \mu_n + \mathcal{O}(\frac{\log\beta}{\beta}) \le \lambda_n(\beta) \le -\Big(\beta + \frac{\gamma_*}{2}\Big)^2 + \mu_n + \mathcal{O}(\frac{\log\beta}{\beta}).$$

The reason is that passing to curvilinear coordinates in the vicinity of the boundary we get in the one-sided case a boundary term containing γ. If we want estimates with separated variables we have to employ rough bounds with γ^* and γ_*. However, the lower bound can be improved by a variational technique; this yields at least the first term in the expansion:

Theorem (E-Minakov-Parnovski'14)

In the asymptotic regime $\beta \to +\infty$ the j-th eigenvalue behaves as

$$\lambda_j(\beta) = -\beta^2 - \gamma^*\beta + \mathcal{O}\big(\beta^{2/3}\big).$$

A proof sketch

We employ variational estimate with trial functions

$$\hat{\varphi}(s,u) = \chi_\varepsilon(s)\Big(\mathrm{e}^{-\alpha u} - \mathrm{e}^{-2a\alpha+u\alpha}\Big),$$

where χ_ε is a smooth function on $[0,L]$ with the support located in an ε-neighborhood of a point s^* in which $\gamma(s^*) = \gamma^*$.

We consider functions of the form

$$\chi_\varepsilon(s) := \chi\Big(\frac{s-s^*+\varepsilon}{2\varepsilon}\Big),$$

where $\chi(x)$ is a fixed smooth function on $\mathbb{R}$ supported in the interval $(0,1)$.

Optimizing the bound by choosing $\varepsilon = \beta^{-1/3}$, we get

$$\frac{b^D_{a,\beta}[\hat{\varphi}]}{\|\hat{\varphi}\|^2_{L^2(0,L)}} \le -\Big(\beta + \frac{\gamma^*}{2}\Big)^2 + \mathcal{O}\big(\beta^{2/3}\big).$$

Proof sketch, continued

This proves the result for the ground state eigenvalue $\lambda_1(\beta)$.

For the higher eigenfunctions we proceed in the same way, using trial functions of the form

$$\hat{\varphi}_j(s,u) = \chi_{\varepsilon,j}(s)\big(\mathrm{e}^{-\alpha u} - \mathrm{e}^{-2a\alpha+u\alpha}\big),$$

where the longitudinal part is constructed from a shifted function χ, for instance

$$\chi_{\varepsilon,j}(s) := \chi\Big(\frac{s-s^*+(2j-1)\varepsilon}{2\varepsilon}\Big).$$

The estimates remain essentially the same, up to the values of the constants involved. By construction, the functions $\chi_{\varepsilon,j}$ with different values of j have disjoint supports, hence $\hat{\varphi}_j$ is orthogonal to $\hat{\varphi}_i$, $i=1,\dots,j-1$, and by the min-max principle the eigenvalue $\lambda_j(\beta)$ has again the stated upper bound. $\square$

Improvements and generalizations

The technique can be further refined using quasimodes for the lower bounds. Moreover, the result can be extended to Robin domains in $\mathbb{R}^d$:

Theorem (Pankrashkin-Popoff'15)

Let H_β be the Robin Laplacian in open, connected domain $\Omega \subset \mathbb{R}^d$, $d \geq 2$. Its j-th the eigenvalue behaves in the limit $\beta \to \infty$ as

$$\lambda_j(\beta) = -\beta^2 + E_j(-\Delta_S - \beta(d-1)H + \mathcal{O}\big(\log\beta\big)\,,$$

where $-\Delta_S$ is the Laplace-Beltrami operator on $S := \partial\Omega$ and H is the mean curvature of the boundary, $(d-1)H = \kappa_1 + \cdots + \kappa_{d-1}$. In particular, if Ω has a compact C^2 boundary, then

$$\lambda_j(\beta) = -\beta^2 - \beta(d-1)H_{\max} + o(\beta)\,.$$

The error term can be further improved if $\partial\Omega$ is more regular.

Improvements and generalizations

Note that for $d = 3$ the *difference between the one- and two-sided situation* is seen: in the Robin case the 'effective potential' is given by the mean curvature only, while for Schrödinger operators it is a combination of Gauss and mean curvatures, $K - M^2$.

The error term in the above result is still too large to allow to distinguish individual eigenvalues. This can be changed, for $d = 2$ at least, if stronger assumptions are imposed:

Theorem (Helffer-Kachmar'15)

Consider $\Omega \subset \mathbb{R}^2$ with a C^∞ smooth boundary, possibly infinite. Suppose that the curvature κ attains its maximum $\kappa_{\max}$ at a unique point, and the maximum is non-degenerate, i.e. $k_2 := -\kappa''(0) > 0$. Then for any positive n there exists a sequence $\{\zeta_{j,n}\}$ such that, for any positive M, the n-th eigenvalue has for $\beta \to \infty$ the following asymptotic expansion

$$\lambda_n(\beta) = -\beta^2 - \kappa_{\max}\beta + (2n-1)\sqrt{\frac{k_2}{2}}|\beta|^{1/2} + \sum_{j=0}^{M} \zeta_{j,n}|\beta|^{\frac{1-j}{4}} + |\beta|^{\frac{1-M}{4}} o(1)$$

A detour from the detour

We note that a part of theses results can be extended to *nonlinear* eigenvalue problems, specifically to the question about the spectral bottom of the *p-Laplacian with Robin boundary conditions*,

$$-\Delta_p u = \Lambda |u|^{p-2} u \quad \text{in } \Omega\,, \quad |\nabla u|^{p-2} \frac{\partial u}{\partial n} = \beta |u|^{p-2} u \quad \text{at } \partial\Omega\,,$$

where Δ_p is the p-Laplacian, $\Delta_p u = \nabla \cdot (|\nabla u|^{p-2} \nabla u)$ and n is the outer unit normal. We ask about the smallest Λ satisfying the above equation, i.e.

$$\Lambda(\Omega, p, \beta) := \inf_{0 \neq u \in W^{1,p}(\Omega)} \frac{\int_\Omega |\nabla u|^p \,\mathrm{d}x - \beta \int_{\partial\Omega} |u|^p \,\mathrm{d}\sigma}{\int_\Omega |u|^p \,\mathrm{d}x}\,.$$

The detour from the detour, continued

We call a domain $\Omega \subset \mathbb{R}^\nu$, $\nu \geq 2$, admissible if

- the boundary $\partial\Omega$ is $C^{1,1}$, i.e. is locally the graph of a function with a Lipschitz gradient
- the principal curvatures of $\partial\Omega$ are essentially bounded
- the map $\partial\Omega \times (0,\delta) \ni (s,t) \mapsto s - tn(s) \in \{x \in \Omega :\ \mathrm{dist}(x,\partial\Omega) < \delta\}$ is bijective for some $\delta > 0$

The mean curvature H of $\partial\Omega$ is, as above, the arithmetic mean of the principal curvatures, and we set $H_{\max} \equiv H_{\max}(\Omega) := \sup\mathrm{ess}\, H$

Theorem (Kovařík-Pankrashkin'16)

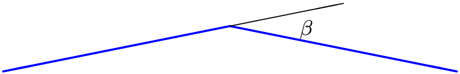
For any admissible domain $\Omega \subset \mathbb{R}^\nu$, $\nu \geq 2$ and any $p \in (1,\infty)$ we have

$$\Lambda(\Omega, p, \beta) = -(p-1)\beta^{p/(p-1)} - \beta(\nu-1)H_{\max}(\Omega) + o(\beta)$$

as $\beta \to \infty$.

Back to the main topic: weakly bent curves

The strong coupling regime is not the only asymptotic problem the leaky structure can offer. Let us turn to *geometric perturbations*.



The simplest example is a *broken line* $\Gamma = \Gamma_\beta$ with a small angle β.

By the above mentioned result the Hamiltonian has an eigenvalues, a single one for small β, and by a simple scaling argument together with an analogy with bent Dirichlet tubes lead us to conjecture that

$$\lambda(H_{\Gamma_\beta}) = -\frac{1}{4}\alpha^2 + a\beta^4 + o(\beta^4)$$

with some $a < 0$ for $\beta \to 0+$.

The question now is (a) what is the coefficient a, and (b) *whether a similar formula holds for more general slightly bent curves*.

Weakly bent curves, continued

Let us first specify the class of curves we shall consider: Γ will be a continuous and piecewise C^2 infinite planar curve without self-intersections parametrized by its arc length, i.e. the graph of a piecewise C^2-smooth function $\Gamma : \mathbb{R} \to \mathbb{R}^2$ such that $|\dot\gamma(s)| = 1$. Moreover,

- there exists a $c \in (0,1)$ such that $|\Gamma(s) - \Gamma(s')| \geq c|s - s'|$ holds for $s, s' \in \mathbb{R}$,
- there are real numbers $s_1 > s_2$ and straight lines Σ_i, $i = 1, 2$, such that Γ coincides with Σ_1 for $s \geq s_1$ and with Σ_2 for $s \leq s_2$,
- one-sided limits of $\dot\gamma$ exists at the points where the function $\ddot\gamma$ is discontinuous.

In particular, the signed curvature $k(s) = \dot\gamma_2(s)\ddot\gamma_1(s) - \dot\gamma_1(s)\ddot\gamma_2(s)$ is piecewise continuous and the one-sided limits of $\dot\gamma$, i.e. *tangent vectors* to the curve at the points of discontinuity exist. We denote them as $\Pi = \{p_i\}_{i=1}^{\sharp\Pi}$ and shall speak of them as of vertices. Consequently, Γ consists of $\sharp\Pi + 1$ simple arcs or *edges*, each having as its endpoints one or two of the vertices.

Weakly bent curves, continued

The curvature integral describes *bending* of the curve. Specifically, the angle between the tangents at the points $\Gamma(s)$ and $\Gamma(s')$ equals

$$\phi(s,s') = \sum_{p_i\in(s,s')} c(p_i) + \int_{(s,s')\setminus\Pi} k(\zeta)\,\mathrm{d}\zeta\,,$$

where $c(p_i)\in(0,\pi)$ is the exterior angle of the two adjacent edges of Γ meeting at the vertex p_i.

Alternatively, we can understand $\phi(s,s')$ as the integral over the interval (s,s') of $\tilde{k}:\ \tilde{k}(s) = k(s) + \sum_{p\in\Pi} c(p)\,\delta(s-p)$. By assumption k, $\tilde{k}$ are compactly supported, thus $\phi(s,s')$ has the same value for all $s<s_2$ and $s_1<s'$ which we shall call the *total bending*.

One can reconstruct Γ from $\tilde{k}$, uniquely up to Euclidean transformations,

$$\Gamma(s) = \left(\int_0^s \cos\phi(u,0)\,\mathrm{d}u\,, \int_0^s \sin\phi(u,0)\,\mathrm{d}u\right).$$

Weakly bent curves, continued

Now we introduce the one-parameter family of 'scaled' curves Γ_β,

$$\Gamma_\beta(s) = \left(\int_0^s \cos \beta\phi(u,0)\,\mathrm{d}u\,, \int_0^s \sin \beta\phi(u,0))\,\mathrm{d}u \right), \quad |\beta| \in (0,1]\,.$$

Note that depending on (non)vanishing of the total bending of Γ the limit $\beta \to 0+$ may have a different meaning, say 'straightening' or 'flattening'.

Next we define an integral operator $A:\ L^2(\mathbb{R}) \to L^2(\mathbb{R})$ through its kernel,

$$\mathcal{A}(s,s') := \frac{\alpha^4}{32\pi} K_0'\left(\frac{\alpha}{2}|s-s'|\right) \left(|s-s'|^{-1} \left(\int_{s'}^s \phi \right)^2 - \int_{s'}^s \phi^2 \right).$$

Lemma

Under the stated assumptions, we have $\int_{\mathbb{R}\times\mathbb{R}} \mathcal{A}(s,s')\,\mathrm{d}s\,\mathrm{d}s' < \infty$.

Weakly bent curves, the result

Now we are in position to state the weak-bending result.

Theorem (E-Kondej'16)

There is a $\beta_0 > 0$ *such that for any* $\beta \in (-\beta_0, 0) \cup (0, \beta_0)$ *the operator* H_{Γ_β} *has a unique eigenvalue* $\lambda(H_{\Gamma_\beta})$ *which admits the asymptotic expansion*

$$\lambda(H_{\Gamma_\beta}) = -\frac{\alpha^2}{4} - \left(\int_{\mathbb{R}\times\mathbb{R}} \mathcal{A}(s,s')\,\mathrm{d}s\,\mathrm{d}s' \right)^2 \beta^4 + o(\beta^4)\,.$$

Proof is laborious but the idea is simple. It is based again on application of the Birman-Schwinger principle which says that

$$-\kappa^2 \in \sigma_{\mathrm{d}}(H_{\Gamma_\beta}) \quad \Leftrightarrow \quad \ker(I - \alpha Q_{\Gamma_\beta}(\kappa)) \neq \emptyset\,,$$

where $Q_{\Gamma_\beta}(\kappa)$ is the integral operator with the kernel

$$\mathcal{Q}_{\Gamma_\beta}(\kappa; s, s') = \frac{1}{2\pi} K_0(\kappa|\gamma_\beta(s) - \gamma_\beta(s')|)\,;$$

moreover, we have $\dim\ker(H_{\Gamma_\beta} + \kappa^2) = \dim\ker(I - \alpha Q_{\Gamma_\beta}(\kappa))$.

Weakly bent curves, continued

One has to compare with the Birman-Schwinger operator corresponding to the *straight line* which has the kernel $K_0\left(\frac{\kappa}{2}|s-s'|\right)$ in the vicinity of the point $\kappa = \frac{1}{2}\alpha$ corresponding to threshold of the essential spectrum.

Let us return to the *broken-line example*: in this case $\mathcal{A}(s,s')$ can be found easily, it vanishes if s, s' have the same sign, being otherwise

$$\mathcal{A}(s,s') = \frac{\alpha^4}{32\pi} K_0'\left(\frac{\alpha}{2}|s-s'|\right) \frac{|ss'|}{|s-s'|}\, \chi_\Omega(s,s')\,,$$

where $\chi_\Omega(\cdot,\cdot)$ is the characteristic function of the set Ω, the union of the second and fourth quadrant. The integral of $\mathcal{A}(s,s')$ over the both variable can be computed explicitly giving

$$\frac{-\frac{1}{4}\alpha^2 - \lambda(H_{\Gamma_\beta})}{-\frac{1}{4}\alpha^2} = -\frac{1}{9\pi^2}\beta^4 + o(\beta^4)\,.$$

Systems with infinite discrete spectrum

One can encounter still another type of asymptotic formulæ in situations when $\sharp\sigma_{\mathrm{disc}}(H_{\alpha,\Gamma} = \infty$. The eigenvalues then typically *accumulate at the bottom of the essential spectrum* and one can ask how fast this accumulation proceeds for a given geometry.

The first question is whether an infinite discrete spectrum may exist. In examples such as the the *broken line in the plane* Γ_β considered above it is not the case: the number of the bound state can be made large for a sharp break, $\pi - \beta$ sufficiently small, but it remains finite.

Nevertheless, examples of infinite discrete spectrum exist. This happens, for instance if $d = 3$ and $\Gamma = \mathcal{C}_\theta$ is the *conical surface* of the opening angle 2θ, in other words

$$\mathcal{C}_\theta := \left\{(x, y, z) \in \mathbb{R}^3 :\ z := \cot(\theta)\sqrt{x^2 + y^2}\right\}, \quad \theta \in (0, \tfrac{1}{2}\pi)\,.$$

The conical layer spectrum

Theorem (Behrndt-E-Lotoreichik'14)

For any $\theta \in (0, \frac{1}{2}\pi)$ and $\alpha > 0$ the essential spectrum of the operator $H_{\alpha,\mathcal{C}_\theta}$ is $[-\frac{1}{4}\alpha^2, \infty)$, the discrete spectrum is infinite and accumulates to $-\frac{1}{4}\alpha^2$.

Proof sketch: The argument proceeds in several steps

- Using the *cylindrical symmetry* one can perform a partial-wave decomposition and observe that only the s-wave component is important, the spectra of the components with nonzero angular momentum are contained in $[-\frac{1}{4}\alpha^2, \infty)$.
- The problem is thus reduced to two dimensions in a halfplane, $(r, z) \in \mathbb{R}_+ \times \mathbb{R}$, using reduced wave functions, $\psi(r, \varphi, z) = \frac{\omega(r,z)}{\sqrt{2\pi r}}$. We introduce rotated coordinates, s along the halfline representing the surface and t perpendicular to it.

Proof sketch, continued

- To check that $\sigma_{\mathrm{ess}}(H_{\alpha,\mathcal{C}_\theta}) \supset [-\frac{1}{4}\alpha^2, \infty)$ we construct a suitable Weyl sequence. It can be done, e.g., using

$$\omega_{n,p}(s,t) := \frac{1}{\sqrt{n}}\Big(\chi_1\big(\tfrac{s}{n}\big)\exp(\mathrm{i}ps)\Big)\Big(\chi_2\big(\tfrac{t}{n}\big)\exp(-\tfrac{\alpha}{2}|t|)\Big)\,,$$

  where χ_1, χ_2 are suitable C_0^∞ functions.

- The check the opposite inclusion, one uses Neumann bracketing taking a symmetric surface *layer neighbourhood* of the width $2\sqrt{n}$ cut at a distance from the cone tip, $s > n$. Its complement does not contribute to the essential spectrum; choosing n large enough, one can make the influence of the term $-(4r(z))^{-1}$ in the Hamiltonian small and to prove in this way that $\inf \sigma_{\mathrm{ess}}(H_{\alpha,\mathcal{C}_\theta}) \geq -\frac{1}{4}\alpha^2 - \varepsilon$ holds for any $\varepsilon > 0$ which yields the result.

Proof sketch, continued

- For the discrete spectrum part we chose suitable trial functions, e,g.,

$$\omega_n(s,t) := \tfrac{1}{n}\chi_1\big(\tfrac{s-n}{n^2}\big)\chi_2\big(\tfrac{t}{\sqrt{n}}\big)\exp\big(-\tfrac{\alpha}{2}|t|\big) \in H_0^1(\mathbb{R}_+^2)\,,$$

where χ_1, χ_2 are again suitable C_0^∞ functions.

- Choosing the indices n appropriately, we can construct a sequence of functions with disjoint supports and prove in this way that the discrete spectrum is infinite and the eigenvalues λ_k satisfy

$$\lambda_k \le -\frac{\alpha^2}{4} - \frac{\gamma(\theta)}{n_k^4}\,, \quad k \in \mathbb{N}\,,$$

where $\gamma(\theta) > 0$ with $n_{k+1} := n_k^2 + n_k$ and $n_1 = N$ with $N \in \mathbb{N}$ sufficiently large. $\square$

Remarks: • The claim remains true if the cone is *locally deformed*.

• $\sigma_{\rm disc}(H_{\alpha,\mathcal{C}_\theta}) = \emptyset$ holds if $d \ge 4$, cf. [Lotoreichik–Ourmières-Bonafos'16].

Accumulation asymptotics

We denote conventionally $\mathcal{N}_E(T) = \sharp\{k \in \mathbb{N} :\ \lambda_k(T) < E\}$, i.e. the counting function of eigenvalues of the operator T below the threshold of its essential spectrum.

Theorem (Lotoreichik–Ourmières-Bonafos'16)

For the conical layer the discrete spectrum accumulates as

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

Proof idea is to estimate the discrete spectrum from above and below using a suitable one-dimensional operator, in this case $-\frac{\mathrm{d}^2}{\mathrm{d}x^2} - \frac{1}{4\sin^2\theta}\,\frac{1}{x^2}$ on the interval $(1,\infty)$ the spectral asymptotics of which is known. This is combined with the estimates on the δ-interaction eigenvalue on an interval with Dirichlet or Neumann boundary similar to those used in the discussion of the strong coupling asymptotics above.

Open questions

In my view, the main challenge concerns the strong-coupling behavior in situations with *less regularity*, in the first place such a behavior for Hamiltonians of *branched leaky graphs.*

Conjecture: In the 'two-sided' situation the strong coupling limit of broken curves/branched graphs behaves *similarly to shrinking Dirichlet networks or tubes*, i.e. a nontrivial limit with the natural energy renormalization can be obtained provided the system exhibits a *threshold resonance*.

The 'one-sided' case is different: recall also that if the 'attractive' Robin billiard has corners of angles $2\theta_j$, the ground state behaves in the limit $\beta \to \infty$ as $-\beta^2 \max_j \left(\sin^{-2} \theta_j \right)$ – cf. [Levitin-Parnovski'08]. Tunneling between the corners was discussed recently by Helffer and Pankrashkin.

Other problems: for *periodic manifolds:* absolute continuity of the spectrum not proven generally, strong-coupling asymptotic behavior of gaps, *magnetic fields:* how do they influence curvature-induced bound states? We conjecture they may destroy them. Furthermore, where does the *mobility edge* lies if Γ is randomized?, etc., etc.

The talk was based, in particular, on

[Ex08] For results prior to 2008 I refer to P.E: Leaky quantum graphs: a review, *Proceedings of the Isaac Newton Institute programme "Analysis on Graphs and Applications"*, AMS "Proceedings of Symposia in Pure Mathematics" Series, vol. 77, Providence, R.I., 2008; pp. 523–564.

[BEL14] J. Behrndt, P.E., V. Lotoreichik: Schrödinger operators with δ-interactions supported on conical surfaces, *J. Phys. A: Math. Theor.* **47** (2014), 355202

[DEKP16] J. Dittrich, P.E., Ch. Kühn, K. Pankrashkin: On eigenvalue asymptotics for strong δ-interactions supported by surfaces with boundaries, *Asympt. Anal.* (2016) **97** (2016), 1–25.

[EJ13] P.E., M. Jex: Spectral asymptotics of a strong δ' interaction on a planar loop, *J. Phys. A: Math. Theor* **46** (2013), 345201.

[EJ14] P.E., M. Jex: Spectral asymptotics of a strong δ' interaction supported by a surface, *Phys. Lett.* **A378** (2014), 2091–2095.

[EK15] P.E., S. Kondej: Gap asymptotics in a weakly bent leaky quantum wire, *J. Phys. A: Math. Theor.* **48** (2015), 495301

[EK16] P.E., S. Kondej: Strong coupling asymptotics for Schrödinger operators with an interaction supported by an open arc in three dimensions, *Rep. Math. Phys.* **77** (2016), 1–17.

[EP14] P.E., K. Pankrashkin: Strong coupling asymptotics for a singular Schrödinger operator with an interaction supported by an open arc, *Comm. PDE* **39** (2014), 193–212.

as well as the other papers mentioned in the course of the presentation.

It remains to say

Thank you for your attention!