Guided quantum dynamics

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Leaky quantum graphs and their generalizations

Let us turn to the *other quantum graph weakness* mentioned in the opening and look for an alternative. The model to examine now is based on singular Schrödinger operators that can formally written as

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

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

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

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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,

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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*

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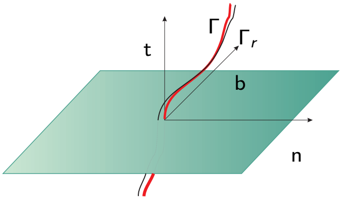
We employ *Frenet's frame* $(t(s), b(s), n(s))$ for Γ. Given $\xi, \eta \in \mathbb{R}$, we set $r = (\xi^2+\eta^2)^{1/2}$ and define family of 'shifted' curves



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

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

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

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

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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

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

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

Spectral analysis: Birman-Schwinger principle

Theorem (Birman-Schwinger principle)

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

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For 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 $(H_0 + \kappa^2)^{-1}(\cdot,\cdot)$.

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

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

where s is the arc length of the curve Γ.

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

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

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

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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.

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

A δ-interaction supported by infinite curves

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

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

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

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

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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

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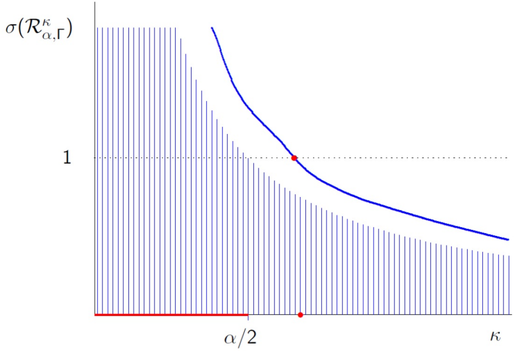
- The best way to illustrate the main steps of the proof is to draw the spectrum of Birman-Schwinger operator in dependence on the spectral parameter κ.

Pictorial sketch of the proof



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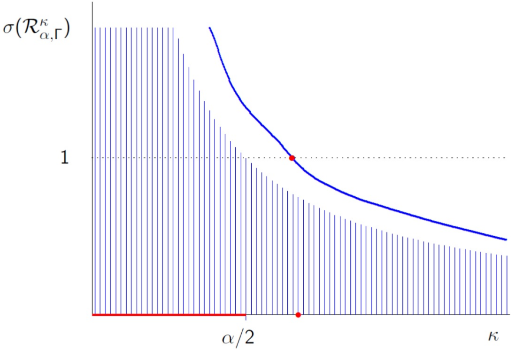

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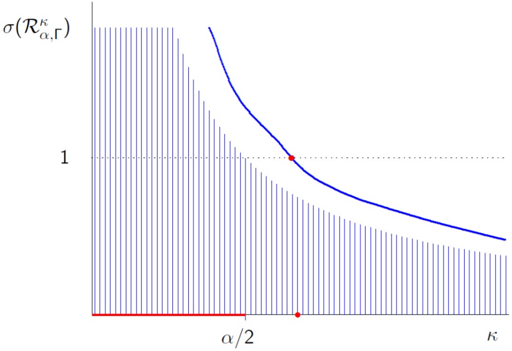

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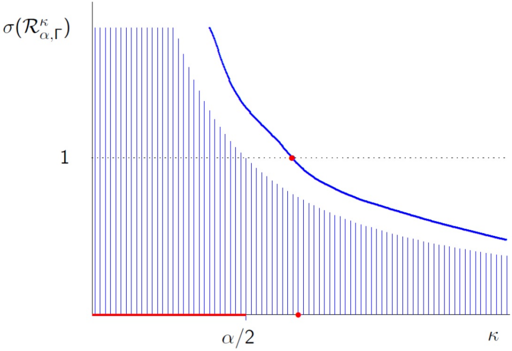

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- from the asymptotic straightness, the perturbation is *compact* so that the 'added' spectrum consists of eigenvalues at most
- the spectrum depends *continuously* on κ and *shrinks to zero* as $\kappa \to \infty$, hence there is a crossing *to the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

Geometrically induced bound states, continued

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

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

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

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

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

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

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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:

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- the 'target' coupling strength α is *any L^∞ function* on Γ, modulo some technical assumptions.

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

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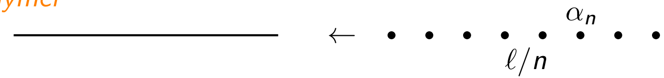
To guess how the coupling parameters of the point interaction should be chosen one can compare $H_{\alpha,\Gamma}$ for a straight Γ with the solvable model of a *straight-polymer*



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

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Theorem

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

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

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

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

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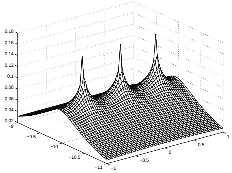

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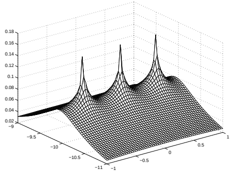

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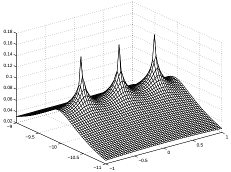

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- There is a trick: consider approximation of $\epsilon\Delta^2 - \Delta - \alpha\delta(x - \Gamma)$ and then take $\epsilon \to 0$; this gives a *norm-resolvent* convergence.

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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?

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

An example: a bottleneck curve

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

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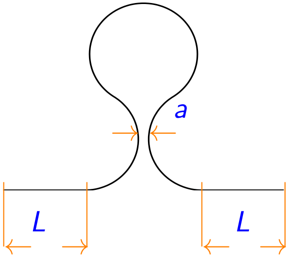

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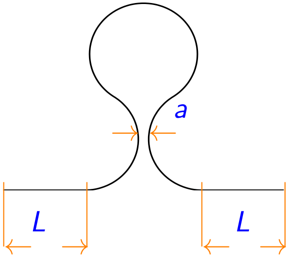

If Γ is a straight line, the transverse eigenfunction is $\mathrm{e}^{-\alpha|y|/2}$, hence the distance at which tunneling becomes significant is $\approx 4\alpha^{-1}$. In the example, we choose $\alpha = 1$.

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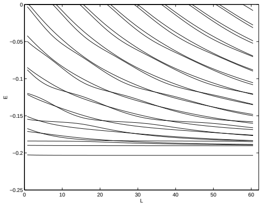

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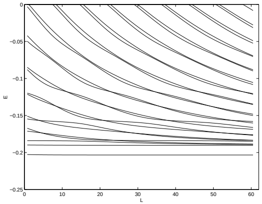

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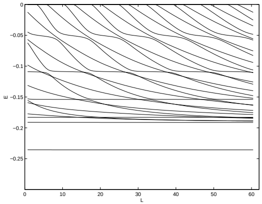

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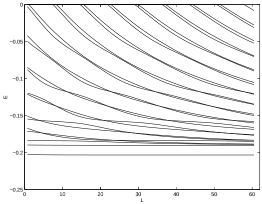

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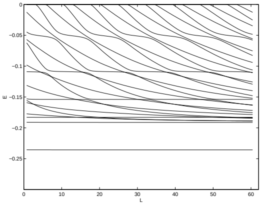

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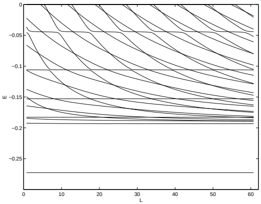

Even narrower one, $a = 1.9$

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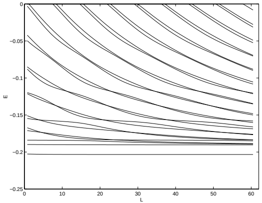
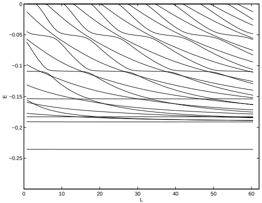
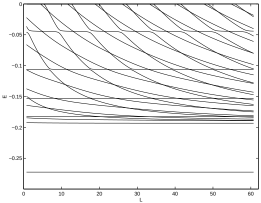


Wide bottleneck, $a = 5.2$



Narrow bottleneck, $a = 2.9$



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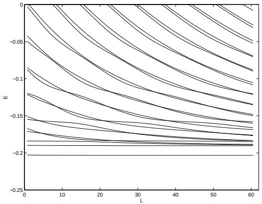

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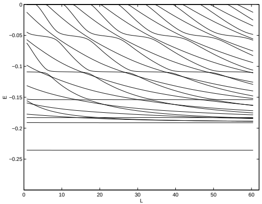

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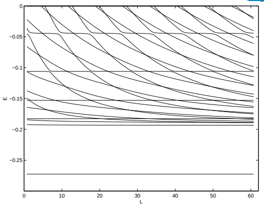

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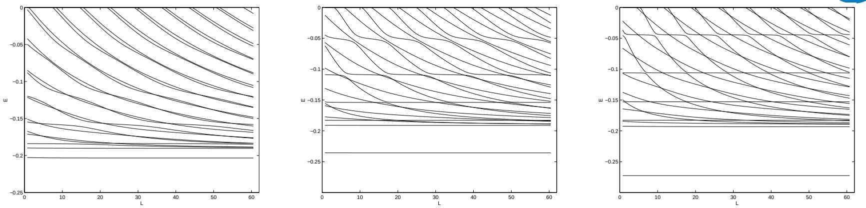

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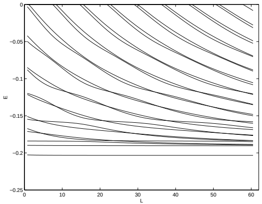

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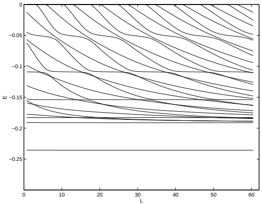

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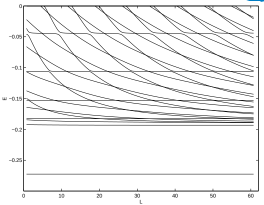

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On the other hand, such a potential represents a way through which the conventional and leaky graphs are related. This will be our next topic.

Strong δ interaction asymptotics

If the *attraction is strong* the motion is strongly localized transversally and the geometry of Γ can be manifested in the discrete spectrum of the operator $H_{\alpha,\Gamma} = -\Delta - \alpha\delta(x - \Gamma)$.

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Theorem

Let Γ be a C^4 smooth curve in $\mathbb{R}^2$ without ends, either a closed loop or infinite, asymtotically straight and without 'near crossings'. In the limit $\alpha \to \infty$ the jth 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 jth eigenvalue of $S_\Gamma = -\frac{\mathrm{d}^2}{\mathrm{d}s^2} - \frac{1}{4}\kappa(s)^2$ on $L^2(0, |\Gamma|)$ or $L^2(\mathbb{R})$, respectively, where κ is curvature of Γ.

P.E., K. Yoshitomi: Asymptotics of eigenvalues of the Schrödinger operator with a strong δ-interaction on a loop, *J. Geom. Phys.* **41** (2002), 344–358.

Strong δ interaction asymptotics

Note that the restriction made were essential. Consider two halflines meeting at a *non-straight angle*. We know that $\sigma_{\mathrm{disc}}(H_{\alpha,\Gamma}) \neq \emptyset$ and in view of the *self-similarity* of Γ, a simple scaling argument shows that its eigenvalues behave as $c\alpha^2$ with some $c < -\frac{1}{4}$ with respect to α.

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Furthermore, if curve Γ has a *cusp* of degree $p > 1$, that is, it is locally homothetic to the graph of the function $f(x) = |x|^{1/p}$, the strong coupling asymptotics of the jth eigenvalue is

$$\lambda_j(\alpha) = -\alpha^2 + c_j(p)\alpha^{\frac{6}{p+2}} + \mathcal{O}\big(\alpha^{\frac{6}{p+2}-\eta_p}\big),$$

where $c_j(p)$ and η_p are (explicitly known) positive constants.

B. Flamencourt, K. Pankrashkin: Strong coupling asymptotics for δ-interactions supported by curves with cusps, *J. Math. Anal. Appl.* **491** (2020), 124287.

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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 $-\frac{1}{4}\alpha^2$ by $\epsilon_\alpha = -4\,\mathrm{e}^{2(-2\pi\alpha+\psi(1))}$.

P.E., S. Kondej: Strong-coupling asymptotic expansion for Schrödinger operators with a singular interaction supported by a curve in $\mathbb{R}^3$, *Rev. Math. Phys.* **16** (2004), 559–582.

Strong δ interaction asymptotics

- For a *surface 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.

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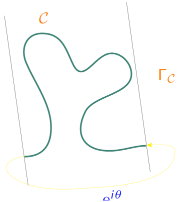
In a similar way one can treat *periodic systems* using the *Bloch* (Floquet, Gel'fand) decomposition: there is a unitary $\mathcal{U}$ such that $\mathcal{U} H_{\alpha,\Gamma} \mathcal{U}^{-1} = \int_{[0,2\pi)^r}^{\oplus} H_{\alpha,\theta}\, \mathrm{d}\theta$ and $\sigma(H_{\alpha,\Gamma}) = \bigcup_{[0,2\pi)^r} \sigma(H_{\alpha,\theta})$.



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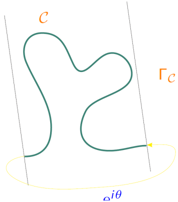
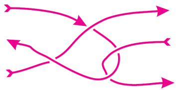


It is important to choose the periodic cells $\mathcal{C}$ of the space and $\Gamma_\mathcal{C}$ of the manifold *consistently*, $\Gamma_\mathcal{C} = \Gamma \cap \mathcal{C}$. Note that $\Gamma_\mathcal{C}$ is not necessarily a 'straight slab', even for $d = 2$, and for $d = 3$ it need not be *simply connected*.



Periodic manifold asymptotics

Theorem

Let Γ be a C^4-smooth r-periodic manifold without boundary. The strong coupling asymptotic behavior of the jth Bloch eigenvalue is

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

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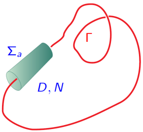
Corollary

If $\dim\Gamma = 1$ *and coupling is strong enough,* $H_{\alpha,\Gamma}$ *has open spectral gaps.*

K. Yoshitomi: Band gap of the spectrum in periodically curved quantum waveguides, *J. Diff. Eqs* **142** (1998), 123–166.

Strong δ interactions: sketch of the argument

Three essential ingredients are involved. The first is *Dirichlet-Neumann bracketing* imposed at the boundary Σ_a of the tubular neighborhood of Γ of radius/halfwidth a, here sketched for a loop in $\mathbb{R}^3$.



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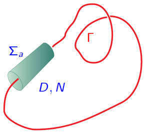

This squeezes $H_{\alpha,\Gamma}$ between a pair of 'disconnected' operators, and since we are interested in *negative eigenvalues*, we have to care about the tube part only because the Dirichlet/Neumann Laplacian in the remaining part of $\mathbb{R}^d$ is *positive*.

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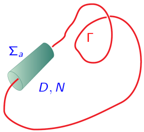

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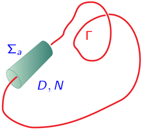

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Then we use inside the tube the *natural curvilinear* (Fermi, parallel) *coordinates* mentioned before, and estimate the coefficients to squeeze $H_{\alpha,\Gamma}$ between operators with *separated variables*. For a curve in $\mathbb{R}^2$, e.g. their *longitudinal* parts are

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

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 operators $U_a^{\pm}$ are *$\mathcal{O}(a)$ close to S_Γ*.

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On the other hand, the *transverse* operators are related to the forms

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

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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

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

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In the other cases the proof is analogous. If $\mathrm{codim}\,\Gamma = 2$ the transverse part is the Dirichlet/Neumann disc of radius r with the point interaction in the center; 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.

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One conjectures that the 'correct' boundary conditions are *Dirichlet*. For a finite planar curve this is indeed the case:

Theorem

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 jth 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 jth 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 $s \in (0, L)$.

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.

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We use again bracketing estimates but now they have to be modified. The *upper* (Dirichlet) one works as before, while for the *lower* (Neumann) one we employ the fact that the arc Γ has by assumption *regular ends*, meaning that it can be extended smoothly in the vicinity of its endpoints.

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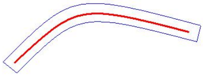
Recall the *generalized Birman-Schwinget principle*; it allows us to express solution to $H_{\alpha,\Gamma}\psi_j = -\mu_j^2\psi_j$ as $\psi_j(x) = \frac{1}{2\pi}\int_\Gamma K_0(\mu_j|x-\Gamma(s)|)\,\phi_j(s)\,\mathrm{d}s$, in other words, as convolutions of the Laplacian Green's function with the corresponding BS eigenfunctions, $\mathcal{R}^{\mu_j}_{\alpha,\Gamma}\phi_j = \phi_j$.

Curves with ends: sketch of the argument

We use again bracketing estimates but now they have to be modified. The *upper* (Dirichlet) one works as before, while for the *lower* (Neumann) one we employ the fact that the arc Γ has by assumption *regular ends*, meaning that it can be extended smoothly in the vicinity of its endpoints.

Recall the *generalized Birman-Schwinget principle*; it allows us to express solution to $H_{\alpha,\Gamma}\psi_j = -\mu_j^2\psi_j$ as $\psi_j(x) = \frac{1}{2\pi}\int_\Gamma K_0(\mu_j|x-\Gamma(s)|)\,\phi_j(s)\,\mathrm{d}s$, in other words, as convolutions of the Laplacian Green's function with the corresponding BS eigenfunctions, $\mathcal{R}^{\mu_j}_{\alpha,\Gamma}\phi_j = \phi_j$.

We choose an *'extended' tubular neighborhood*, at each endpoint longer by $a := \frac{6}{\alpha}\ln\alpha$. Now we *loose the advantage of variable separation* but with the help of the above formula one can check that the Neumann condition imposed at this distance from the curve has an effect which can be included into the error term.



An extended neighbourhood

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

Using a similar argument, just technically a bit more involved, one can obtain asymptotic results for an arc in $\mathbb{R}^3$:

Theorem

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.

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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

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

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

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

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

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.

Surfaces 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, in other words, that there exists a larger C^4-smooth surface Γ_2 such that $\overline{\Gamma} \subset \Gamma_2$.

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We consider again the comparison 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 *Gauss* and *mean* curvatures of Γ

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Theorem

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

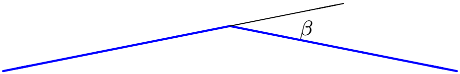
$$\lambda_j(H_{\alpha,\Gamma}) = -\frac{\alpha^2}{4} + \mu_j^D + o(1) \quad \text{as} \quad \alpha \to \infty\,.$$

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

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

Another asymptotics: slightly bent curves

A different asymptotics type concerns weak geometric perturbations. The simplest example is a *broken line* $\Gamma = \Gamma_\beta$ with a small angle β.



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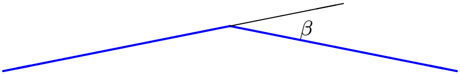

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For slightly bent *Dirichlet tubes* one derives using BS principle that the gap is proportional to the *fourth power* of the bending angle; led by this analogy we conjecture that

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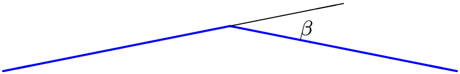

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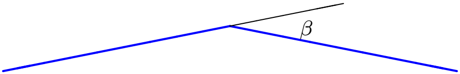

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The question now is (a) what is the coefficient a, and (b) what is the *class of curves* for which such a formula holds.

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,

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

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In particular, the *signed curvature* $\gamma(s) = \dot\Gamma_2(s)\ddot\Gamma_1(s) - \dot\Gamma_1(s)\ddot\Gamma_2(s)$ 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

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

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

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

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One can reconstruct Γ from $\tilde\gamma$, 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,

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

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

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

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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

With these prerequisites, we are finally able to state the sought weak-bending result:

Theorem

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

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P.E., S. Kondej: Gap asymptotics in a weakly bent leaky quantum wire, *J. Phys.* **A48** (2015), 495301

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

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

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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.

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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

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

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$$\Gamma_\beta := \big\{(x_1, x_2, x_3) \in \mathbb{R}^3 \colon x_3 = \beta f(x_1, x_2)\big\} \subset \mathbb{R}^3 \,,$$

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where $f \colon \mathbb{R}^2 \to \mathbb{R}$ is a nonzero *C^2-smooth*, *compactly supported* function and ask how the spectrum of $H_{\alpha,\beta} := -\Delta - \alpha\delta(x - \Gamma_\beta)$ in the asymptotic regime $\beta \to 0+$.

The asymptotic expansion

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Theorem

Let $\alpha > 0$ *be fixed and set*

$$\mathcal{D}_{\alpha,f} := \int_{\mathbb{R}^2} |p|^2 \left(\alpha^2 - \frac{2\alpha^3}{\sqrt{4|p|^2 + \alpha^2} + \alpha} \right) |\hat{f}(p)|^2 \mathrm{d}p > 0 \,,$$

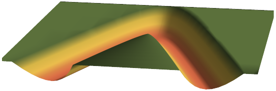
where $\hat{f}$ *is the Fourier transform of* f. *Then* $\#\sigma_{\mathrm{disc}}(H_{\alpha,\beta}) = 1$ *holds for all sufficiently small* $\beta > 0$ *and, moreover,* $\lambda_1^\alpha(\beta)$ *admits the asymptotic expansion*

$$\lambda_1^\alpha(\beta) = -\frac{\alpha^2}{4} - \exp\left(-\frac{16\pi}{\mathcal{D}_{\alpha,f}\beta^2} \right) (1 + o(1)) \quad \textit{as} \;\; \beta \to 0+$$

P.E., S. Kondej, V. Lotoreichik: Asymptotics of the bound state induced by δ-interaction supported on a weakly deformed plane, *J. Math. Phys.* **59** (2018), 013051

Soft quantum waveguides

To remove *both deficiencies* mentioned in the opening of Lecture II we pass to a more realistic model with the δ replaced by a regular *potential well*.



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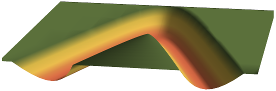

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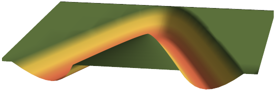

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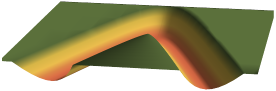

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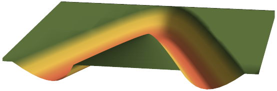

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(c) $|\Gamma(s) - \Gamma(s')| \to \infty$ holds as $|s - s'| \to \infty$ (no U-shapes, etc.).

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

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

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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,

$$x(s, u) = \big(\Gamma_1(s) - u\dot\Gamma_2(s), \Gamma_2(s) + u\dot\Gamma_1(s)\big),$$

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 with an *attractive potential* supported in Ω^a. To this aim, we consider

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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

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

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 $\sigma(H_{\Gamma_0,V}) = \sigma_{\mathrm{ess}}(H_{\Gamma_0,V}) = [\epsilon_0, \infty)$.

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- 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*, $V_\varepsilon: \; V_\varepsilon(u) = \frac{1}{\varepsilon} V\left(\frac{u}{\varepsilon}\right)$

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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 II we can conclude:

Proposition

Let Γ be non-straight and assume that assumptions (a)–(d) are satisfied, then $\sigma_{\rm disc}(H_{\Gamma,V_{J,0}}) \neq \emptyset$ 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,

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- *'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.

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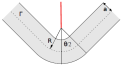

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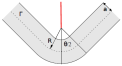

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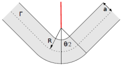

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- Moreover, these results open a plethora of questions about *soft waveguide* properties in different dimensions, different geometries, topological properties of such *potential ditch networks*, etc.

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