Geometrically induced spectrum in soft quantum waveguides

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My topic: geometric effects in the spectrum

A well-known example of such an effect is provided by the Dirichlet Laplacian in $L^2(\Omega)$, where $\Omega \subset \mathbb{R}^d$, $d = 2, 3$, is a *tubular region* the spectrum of which depends on the *geometry of* Ω, e.g., if such a tube is *bent, but asymptotically straight*, we have $\sigma_{\mathrm{disc}}(-\Delta_{\mathrm{D}}^{\Omega}) \neq \emptyset$

There is a number of related results including other dimensions, boundaries, and different geometric perturbations:

P.E., H. Kovařík: *Quantum Waveguides*, Springer, Cham 2015

Analogous effects one can observe in case of *singular Schrödinger operators* formally written as $-\Delta - \alpha\delta(x - \Gamma)$ in $L^2(\mathbb{R}^2)$ with $\alpha > 0$ and Γ being is a curve, a graph, a surface, etc.

If, for instance, Γ is a *non-straight, piecewise C^1-smooth curve* such that $|\Gamma(s) - \Gamma(s')| \geq c|s - s'|$ for some $c \in (0, 1)$ and asymptotically straight in a suitable sense, then $\sigma_{\mathrm{ess}}(-\Delta_{\Gamma,\alpha}) = [-\frac{1}{4}\alpha^2, \infty)$ and the operator has at least one eigenvalue below the threshold $-\frac{1}{4}\alpha^2$.

P.E., T. Ichinose: Geometrically induced spectrum in curved leaky wires, *J. Phys. A: Math. Gen.* **34** (2001), 1439–1450.

Soft quantum waveguides in two dimensions

The main question here is what happens if we replace the singular interaction by a *regular potential channel*. We consider an infinite planar curve $\Gamma: \mathbb{R} \to \mathbb{R}^2$ without self-intersections, parametrized by its arc length s and suppose that

- (a) Γ is C^2-smooth so $\gamma(s) = (\dot\Gamma_2\ddot\Gamma_1 - \dot\Gamma_1\ddot\Gamma_2)(s)$ makes sense,
- (b) γ is either of *compact support*, $\operatorname{supp}\gamma \subset [-s_0, s_0]$ for an $s_0 > 0$, or Γ is *C^4-smooth* and $\gamma(s)$, $\dot\gamma(s)$, $\ddot\gamma(s)$ tend to zero as $|s| \to \infty$,
- (c) $|\Gamma(s) - \Gamma(s')| \to \infty$ holds as $|s - s'| \to \infty$.

Next we define the strip neighborhood of the curve, $\Omega^a := \{x \in \mathbb{R}^2 :\, \operatorname{dist}(x, \Gamma) < a\}$, in particular, $\Omega_0^a := \mathbb{R} \times (-a, a)$ corresponds to a straight line Γ_0, and assume that

- (d) Ω^a *does not intersect itself*, in particular, we have $a\|\gamma\|_\infty < 1$;

points of Ω^a can be uniquely expressed in parallel (Fermi) coordinates,

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

Soft quantum waveguides in two dimensions

This allows us to built a potential 'ditch' in Ω^a considering

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

($V \geq 0$ and $\|V\|_\infty < \infty$ is assumed for convenience only) and putting

$$H_{\Gamma,V} = -\Delta - V(x)\,, \quad V(x) = v(\mathrm{dist}(x,\Gamma))$$

We also introduce the operator $h_V = -\partial_x^2 - V(x)$ on $L^2(\mathbb{R})$ 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 ϵ_0 is simple and associated with a positive $\phi_0 \in H^2(\mathbb{R})$.

Proposition

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

Asymptotic results

Recall that $-\Delta - \alpha\delta(x-\Gamma)$ is obtained as a *norm-resolvent limit* of Schrödinger operators with *scaled regular potentials*, namely $V_\varepsilon:\ V_\varepsilon(u) = \frac{1}{\varepsilon} V\left(\frac{u}{\varepsilon}\right)$; this follows from a general result obtained in

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

Proposition

Let a C^2-smooth curve $\Gamma:\ \mathbb{R} \to \mathbb{R}^2$ satisfy assumption of the above theorem; if $\operatorname{supp}\gamma$ 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.*

Similarly, for a *flat-bottom* waveguide, $v_a(u) = V_0\chi_{[-a,a]}(u)$, we have

Proposition

Suppose that Γ is not straight and assumptions (a)–(d) *are satisfied, then the operator H_{Γ,V_a} referring to the flat-bottom potential has nonempty discrete spectrum for all V_0 large enough.*

Birman-Schwinger analysis

However, one would like to know whether the curvature can induce the existence of discrete spectrum also *beyond the asymptotic regime*.

There are two main ways how to do that: (a) to use *Birman-Schwinger principle*, or (b) variationally, by constructing suitable *trial functions*.

The first way relies on the operator in $L^2(\mathbb{R}^2)$ defined for $z \in \mathbb{C} \setminus \mathbb{R}_+$ by

$$K_{\Gamma,V}(z) := V^{1/2}(-\Delta - z)^{-1}V^{1/2};$$

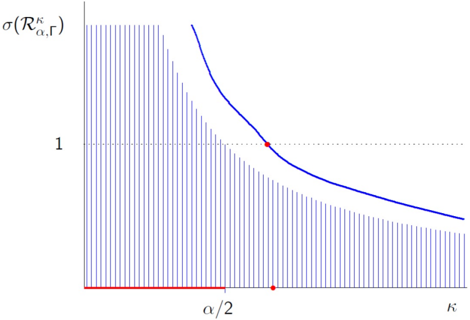
the discrete spectrum of $H_{\Gamma,V}$ can be found using the following claim:

Proposition

$z \in \sigma_{\mathrm{disc}}(H_{\Gamma,V})$ holds if and only if $1 \in \sigma_{\mathrm{disc}}(K_{\Gamma,V}(z))$. The function $\kappa \mapsto K_{\Gamma,V}(-\kappa^2)$ is continuous and decreasing in $(0,\infty)$, tending to zero in the norm topology, that is, $\|K_{\Gamma,V}(-\kappa^2)\| \to 0$ holds as $\kappa \to \infty$

This works well in the singular potential case where the 'sandwiching' of the free resolvent is replaced by taking its trace at the points of Γ.

Recall the BS proof scheme in the singular case



- in the straight case $\sigma(\mathcal{R}^{\kappa}_{\alpha,\Gamma_0}) = [0, \frac{\alpha}{2\kappa}]$ is checked directly
- since $\kappa \mapsto \frac{1}{2\pi} K_0(\kappa|x-x'|)$ is *decreasing*, the perturbation is *sign-definite*; it is not difficult to check that $\sup \sigma(\mathcal{R}^{\kappa}_{\alpha,\Gamma}) > \frac{\alpha}{2\kappa}$
- 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 $\frac{1}{2}\alpha$

Existence of bound states

Since v is *compactly supported* we can use Fermi coordinates to 'straighten' the strip and consider again the bending as a perturbation on Ω_0^a, however, its sign-definiteness is now an *assumption*; this yields the following sufficient condition for the discrete spectrum existence:

Theorem

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

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

for all (s,u), $(s',u')\in\Omega_0^a$, *then we have* $\sigma_{\mathrm{disc}}(H_{\Gamma,V})\neq\emptyset$ *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.

Remarks

• In contrast to the above asymptotic results, the condition has a quantitative character, however, the integral on the positivity of which it relies may not not easy to evaluate generally.

• The sufficient condition for the discrete spectrum existence can be extended to soft waveguides in *three dimensions* under the assumption that profile potential V is *rotationally symmetric* w.r.t. the tube axis.

• If it is not the case, the result still holds if the channel profile is fixed in a particular frame which is, modulo technicalities, the one which *rotates w.r.t. the Frenet frame* of the generating curve Γ and the *angular velocity* of this rotation coincides with the *torsion* of Γ.

P.E.: Soft quantum waveguides in three dimensions, *J. Math. Phys.* **63** (2022), 042103

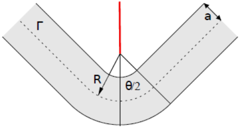
• If this condition is not satisfied, the problems is open; recall that for *Dirichlet tubes* twisting gives rise to an effective *repulsive* interaction.

T. Ekholm, H. Kovařík, D. Krejčiřík: A Hardy inequality in twisted waveguides, *Arch. Rat. Mech. Anal.* **188** (2008), 245–264.

Variational approach

An alternative to Birman-Schwinger is to apply variational estimates to the original operator $H_{\Gamma,V}$. The trouble is to find a suitable trial function which – in contrast to Dirichlet tubes where this approach works well – is that such a function is now *supported in the whole plane/space*.

The only prior result in the literature concerned a simple example of the so-called *bookcover-shaped* potential ditch localized in the following Ω^a:



Source: the cited paper

S. Kondej, D. Krejčiřík, J. Kříž: Soft quantum waveguides with a explicit cut locus, *J. Phys. A: Math. Theor.* **54** (2021), 30LT01

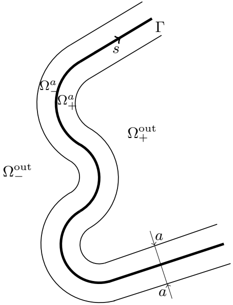
The potential here is not assumed to be nonnegative and may be arbitrarily shallow. Note also that the generating curve here is not C^2.

Our next aim is to show that using variational approach we can go far beyond the bookcover example of [KKK'21]

The existence: more complicated guides

We adopt the following assumptions:

- (s1) Γ is *C^1-smooth* and *piecewise C^3*, *non-straight* but *straight outside a compact*; its curved part consists of a finite number of segments such that on each of them the monotonicity character of the signed curvature $\kappa(\cdot)$ of Γ and its sign are preserved,
- (s2) $|\Gamma(s_+) - \Gamma(s_-)| \to \infty$ as $s_\pm \to \pm\infty$,
- (s3) the strip $\Omega^a := \{x \in \mathbb{R}^2 : \mathrm{dist}(x, \Gamma) < a\}$ does not intersect itself.



The potential, including a possible bias

We consider the channel profile operator of the form

$$h := -\frac{\mathrm{d}^2}{\mathrm{d}t^2} + v(t) + V_0 \chi_{[a,\infty)}(t), \quad V_0 \geq 0$$

and use (some of) the following assumptions:

- p1 $v \in L^2(\mathbb{R})$ and $\operatorname{supp} v \subset [-a, a]$,
- p2 sometimes we use *mirror symmetry*, $v(t) = v(-t)$ for $t \in [-a, a]$,
- p3 $\inf \sigma(h)$ is a negative (ground state) eigenvalue μ associated with a real-valued eigenfunction ϕ_0 normalized by $\phi_0(-a) = 1$, or
- p4 operator h has a *zero-energy resonance*, meaning that $h \geq 0$ and $-(1-\varepsilon)\frac{\mathrm{d}^2}{\mathrm{d}t^2} + v(t) + V_0 \chi_{[a,\infty)}(t)$ has a negative eigenvalue for any $\varepsilon > 0$. In that case, equation $h\phi = 0$ has a real-valued solution $\phi_0 \in H^2_{\mathrm{loc}}(\mathbb{R})$ not increasing at infinity; we set again $\phi_0(-a) = 1$.

The soft waveguide Hamiltonian

As before, the object of our interest is the Schrödinger operator

$$H_{\Gamma,V} = -\Delta + V(x)$$

on $L^2(\mathbb{R}^2)$ with the potential defined using the locally orthogonal coordinates (s,t) in the strip as

$$V(x) = \begin{cases} v(t) & \text{if } x \in \Omega^a \\ V_0 & \text{if } x \in \Omega_+ \setminus \Omega^a \\ 0 & \text{otherwise} \end{cases}$$

We drop the subscript of $H_{\Gamma,V}$ if it is clear from the context. We have:

Proposition

Under assumptions (s1)–(s3), (p1) and (p3), the operator is self-adjoint with $D(H_{\Gamma,V}) = H^2(\mathbb{R}^2)$, and $\sigma_{\mathrm{ess}}(H_{\Gamma,V}) = [\mu, \infty)$. If $h \geq 0$, the same is true with $\mu = 0$.

The unbiased case

The zero-energy resonance situation is easier:

Theorem

Assume (s1)–(s3), (p1) and (p4). If $V_0 = 0$ and

$$[\phi_0(a)^2 - \phi_0(-a)^2] \int_{\mathbb{R}} \kappa(s)\, \mathrm{d}s \leq 0$$

holds, then $H_{\Gamma,V}$ has at least one negative eigenvalue.

Recall that $\kappa \neq 0$. The condition is naturally satisfied if $\phi_0(a) = \phi_0(-a)$, in particular, under assumption (p2). The integral equals $\pi - \theta$ where θ is the asymptote angle, hence if $\phi_0(a) \neq \phi_0(-a)$, at least one bound state exists if $\theta = \pi$ or $\theta \in (0, \pi)$ and ϕ_0 is larger at the 'outer' side of Ω^a.

Theorem

Assume (s1)–(s3) and (p1)–(p3). Let further $V_0 = 0$, then $H_{\Gamma,V}$ has at least one eigenvalue below the continuum threshold μ.

P.E., S. Vugalter: Bound states in bent soft waveguides, *J. Spect. Theory*, to appear; `arXiv:2304.14776`

A rough sketch of the proof

We seek a trial function $\psi \in H^1(\mathbb{R}^2)$ such that $Q[\psi] < \mu\|\psi\|^2$, where

$$Q[\psi] = \|\nabla\psi\|^2 + \int_{\Omega^a} v(t)|\psi(x(s,t))|^2 \mathrm{d}s\mathrm{d}t$$

Let us fix the geometry. We choose the origin O of the coordinates so that the asymptotes are symmetric w.r.t. x axis at angles $\pm\theta_0$, and s_0 so that $\Gamma(\pm s)$ there have the *same Euclidean distance from O*.

We begin with *trial function inside the strip* choosing s_0, such that the points $\Gamma(\pm s_0)$ lay outside the curved part of Γ, and $s^* > s_0$, defining

$$\chi_{\mathrm{in}}(s) := \begin{cases} 1 & \text{if } |s| < s_0 \\ \ln\frac{s^*}{|s|}\left(\ln\frac{s^*}{s_0}\right)^{-1} & \text{if } s_0 \le |s| \le s^* \\ 0 & \text{if } s_0 \le |s| \le s^* \end{cases}$$

Recalling that ϕ_0 satisfies $h\phi_0 = \mu\phi_0$, we put

$$\psi(s,t) = \phi_0(t)\chi_{\mathrm{in}}(s) + \nu g(s,t), \quad |t| \le a,$$

where ν and a compactly supported function g will be chosen later.

Sketch of the proof, continued

We denote by $Q_{\rm int}[\psi]$ the contribution from the strip to the shifted form, $Q[\psi]-\mu\|\psi\|^2$; using the parallel coordinates we can write it as

$$Q_{\rm int}[\psi] = \int_{|t|\le a} \Big\{ \Big(\frac{\partial\psi}{\partial s}\Big)^2 (1-\kappa(s)t)^{-1} + \Big(\frac{\partial\psi}{\partial t}\Big)^2 (1-\kappa(s)t) + (v(t)-\mu)|\psi|^2 (1-\kappa(s)t) \Big\}\, \mathrm{d}s\mathrm{d}t.$$

It is quadratic in ν, we can choose g so that *linear term is nonzero*. Denoting for brevity (keeping the bias V_0 for further purposes)

$$\phi_\pm = \phi_0(\pm a), \quad \xi_+ = -\sqrt{|\mu|+V_0}, \quad \xi_- = \sqrt{|\mu|},$$

we can estimate the internal contribution as follows,

$$Q_{\rm int}[\psi] \le -\frac{1}{2}\delta\nu + \left[\xi_+\phi_+^2 - \xi_-\right]\|\chi_{\rm in}\|^2 - \left[\xi_+\phi_+^2 + \xi_-\right] a \int_{\mathbb{R}} \kappa(s)\,\mathrm{d}s + \frac{1}{2}(\phi_+^2 - 1)\int_{\mathbb{R}} \kappa(s)\,\mathrm{d}s + \tau_0^{-1}\|\phi_0\restriction_{[-a,a]}\|^2 \|\chi_{\rm in}'\|^2.$$

where $\tau_: = 1 - a\|\kappa\|_\infty$ and the last term on the right-hand side can be made arbitrarily small choosing $s^* \gg s_0$.

The zero-energy resonance case

If $V_0 = \mu = 0$ we have $\xi_\pm = 0$ and since $(\phi_+^2 - 1)\int_{\mathbb{R}} \kappa(s)\,\mathrm{d}s \le 0$ holds by assumption, the above estimate simply becomes $Q_{\rm int}[\psi] \le -\frac{1}{4}\delta\nu$.

To conclude the proof we have thus to choose the outer part of trial function so that its contribution can be made smaller than any fixed positive number.

If $V_0 = \mu = 0$, we have $\phi_0(t) = \mathrm{const}$ for $|t| \ge a$, and to get an H^1 trial function, we have to multiply this constant (possibly different in $\Omega_\pm$) by a suitable mollifier $\chi_{\rm out}$ of which we require

- in $\mathbb{R}^2 \setminus \Omega^a$ the function depends on $\rho = \mathrm{dist}(x, O)$ only,
- continuity at the boundary of Ω^a: at points $x(s, \pm a)$ the relation $\chi_{\rm out}(x) = \chi_{\rm in}(s)$ holds.

With a bit of computing one can check that the goal is achieved for $s^* \gg s_0$; this concludes the proof of the first theorem.

The case $\mu < 0$

The proof of the second theorem is much more complicated. In view of the symmetry and absence of the bias, we have $\phi_+ = 1$ and $\xi_+ = -\xi_-$. Keeping thus $\psi(s,t) = \phi_0(t)\chi_{\rm in}(s) + \nu g(s,t)$ for the interior part, we have

$$Q_{\rm int}[\psi] \le -\frac{1}{4}\delta\nu - 2|\mu|^{1/2}\|\chi_{\rm in}\|^2.$$

To construct the outer part, we adopt first an additional assumption,

- s4 the curved part of Γ is piecewise C^∞-smooth consisting of a *finite array of circular arcs*; at its endpoints it is C^1-smoothly connected to the halflines,

in other words, the signed curvature $\kappa(\cdot)$ of such a Γ is a step function.

In $\Omega_{\rm out}$ we now define a function with the appropriate exponential decay,

$$\phi(x) := \exp\{-\xi(\mathrm{dist}(x,\Gamma) - a)\}, \quad x \in \mathbb{R}^2 \setminus \Omega^a,$$

where $\xi := \xi_- = -\xi_+ = |\mu|^{1/2}$; the sought trial function will be then of the form $\psi_{\rm out} = \phi\chi_{\rm out}$ with the mollifier $\chi_{\rm out}$ to be specified below.

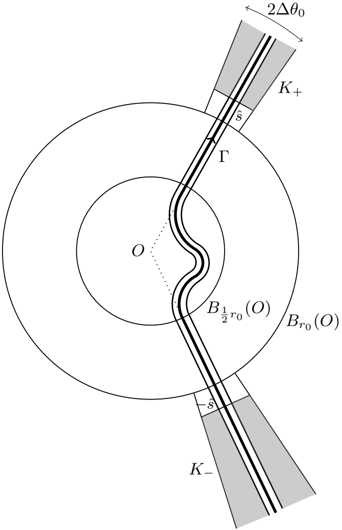
The external mollifier

To construct it, we consider several regions in the plane:

- the disc $B_{\frac{1}{2}r_0}(O)$ containing the curved part of Γ
- the doubled disc $B_{r_0}(O)$ such that $\chi_{\mathrm{out}}(x) = 1$ on $B_{r_0}(O) \setminus \Omega^a$
- disjoint *conical sectors* $K_\pm$ of angle $2\theta_0$ in $\mathbb{R}^2 \setminus B_{r_0}(O)$ centered around the asymptotes of Γ; within them one can use the parallel coordinates and define $\chi_{\mathrm{out}}(s,t) = \chi_{\mathrm{in}}(s)$

In the remaining part of the plane we choose χ_{out} as a *function of the distance ρ from the origin O only*, and such that χ_{out} is *continuous* in Ω_{out}; it is clear that the radial decay of such an external mollifier is determined by the function $\chi_{\mathrm{in}}(s)$

The regions used in the proof



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As usual one has first to check that the mollifier effect in the kinetic part of the quadratic form can be made small. With the above choice we have

$$\int_{\Omega_{\mathrm{out}}} |\nabla\psi_{\mathrm{out}}(x)|^2 \mathrm{d}x \le \int_{\Omega_{\mathrm{out}}} |\nabla\phi(x)|^2 \chi^2_{\mathrm{out}}(x)\, \mathrm{d}x + \mathcal{O}(r_0^{-1}) \quad \text{as} \quad r_0 \to \infty;$$

choosing r_0 large enough, the error term can be made $\frac{1}{8}\delta\nu$ with the $\delta\nu$ we used in estimating the interior part.

Proof sketch, continued

With this choice it is easy to check that

$$\int_{\Omega_{\rm out}\cap\{K_+\cup K_-\}} |\phi(x)\chi_{\rm out}(x)|^2\,\mathrm{d}x \le |\mu|^{-1/2}\|\chi_{\rm in}\|^2_{L^2((-\infty,-\hat{s}]\cup[\hat{s},\infty))}$$

and it remains to estimate the integral over $\Omega_{\rm out}\setminus\{K_+\cup K_-\}$ which can only increase if we remove $\chi_{\rm out}$, hence we have to check that

$$\int_{\Omega_{\rm out}\setminus\{K_+\cup K_-\}} |\phi(x)|^2\,\mathrm{d}x \le 2\hat{s}\,|\mu|^{-1/2} + \frac{1}{16}|\mu|^{-1}\delta\nu,$$

where we have used the fact that $\|\chi_{\rm in}\|^2_{L^2((-\hat{s},\hat{s}))} = 2\hat{s}$.

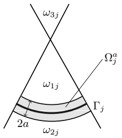
Now we employ the additional assumption (s4). The function $d_x : \mathbb{R}\to\mathbb{R}_+$ defined by $d_x(s) := \mathrm{dist}(x,\Gamma(s))$ is C^1 smooth for any $x\in\mathbb{R}^2$ and *piecewise monotonous* because on each arc it can have at most one extremum. Since $d_x(s)\to\infty$ holds as $s\to\pm\infty$, the function has a *global minimum*, and it may also have a finite number of *local extrema* which come in *pairs*, a minimum adjacent to a maximum.

Proof sketch, continued

Let s_x^0 be the coordinate of the global minimum and s_x^i refer to all the extrema; the index sets $M_x^{\uparrow}$ and $M_x^{\downarrow}$ refer to maxima and minima, respectively. Then for all $x \in \Omega_{\mathrm{out}}$ we obviously have

$$\exp\{-2\xi(d_x(s_x^0) - a)\} \leq -\sum_{s_x^i \in M_x^{\uparrow}} \exp\{-2\xi(d_x(s_x^i) - a)\} + \sum_{s_x^i \in M_x^{\downarrow}} \exp\{-2\xi(d_x(s_x^i) - a)\}$$

We will combine this inequality with some simple geometrical facts:



Proposition

Let Γ_j be one the arcs of Γ and $\omega_{1j}, \omega_{2j}, \omega_{3j}$ and Ω_j^a as in the figure

- (i) *If $x \in \omega_{1j} \cup \omega_{2j}$, then $d_x(\cdot)$ has a minimum in the interior of Γ_j.*
- (ii) *If $x \in \omega_{3j}$, then $d_x(\cdot)$ has a maximum in the interior of Γ_j.*
- (iii) *$x \notin \bar{\omega}_{1j} \cup \bar{\omega}_{2j} \cup \bar{\omega}_{3j} \cup \bar{\Omega}_j^a$, then $d_x(\cdot)$ has no extremum on Γ_j.*
- (iv) *$d_x(\cdot)$ has no more than one critical point in the interior of Γ_j.*
- (v) *If $x \in \omega_{kj}$ for any of $k = 1, 2, 3$, then the one-sided derivative $d_x'(s) \neq 0$ at the endpoints of Γ_j.*

Proof sketch, continued

Within the regions introduced the minimal and maximal distances are easily expressed,

$$d_x(s_x^i) = \mathrm{dist}(x, \Gamma_j) \quad \text{if} \;\; s_x^i \in \Gamma_j \cap M_x^{\downarrow},$$
$$d_x(s_x^i) = |\kappa_j|^{-1} + \mathrm{dist}(x, O_j) \quad \text{if} \;\; s_x^i \in \Gamma_j \cap M_x^{\uparrow}.$$

Thus allows us to replace the right-hand side terms in the above estimate almost everywhere by

$$-\sum_j \exp\{-2\xi(|\kappa_j|^{-1} + \mathrm{dist}(x, O_j) - a)\}\iota_j^3(x) \quad \text{and} \quad \sum_j \exp\{-2\xi(\mathrm{dist}(x, \Gamma_j) - a)\}\iota_j^{1,2}(x),$$

respectively, where $\iota_j^{1,2}$ and ι_j^3 are the appropriate characteristic functions, hence $\int_{\Omega_{\mathrm{out}}\setminus\{K_+\cup K_-\}} \exp\{-2\xi(d_x(s_x^0) - a)\}\,\mathrm{d}x$ is bound from above by

$$\sum_j \int_{(\omega_{1j}\cup\omega_{2j})\cap\{\Omega_{\mathrm{out}}\setminus\{K_+\cup K_-\}\}} \exp\{-2\xi(\mathrm{dist}(x, \Gamma_j) - a)\}\,\mathrm{d}x$$
$$-\sum_j \int_{\omega_{3j}\cap\{\Omega_{\mathrm{out}}\setminus\{K_+\cup K_-\}\}} \exp\{-2\xi(|\kappa_j|^{-1} + \mathrm{dist}(x, O_j) - a)\}\,\mathrm{d}x,$$

where the sums include the straight segments with $|s| > \hat{s}$. There is a *double counting* here as x may belong to different ω_{kj}; this does not matter as long as we consider the contributions referring of a given Γ_j together.

Proof sketch, continued

To simplify the estimate, we note that the last bound can only increase if we replace the integration domains by $(\omega_{1j} \cup \omega_{2j}) \setminus \{K_+ \cup K_-\}$ and $\omega_{3j} \setminus \{K_+ \cup K_-\}$, respectively. This follows from the fact that any fixed j the three regions are in Ω_{out}, i.e. $\omega_{kj_0} \cap \Omega^a_{j_0} = \emptyset$ holds for $k = 1, 2, 3$.

As mentioned, the summation includes the straight parts of Γ; without going into details, one can check that their contribution is estimated by a multiple of $\mathrm{e}^{-\xi \sin 2\Delta\theta_0 \cdot \rho(\hat{s})}$ becoming thus negligible for large r_0.

To get rid of the conical sectors, we note that that the positive part of the estimate cannot decrease if we enlarge the integration domain replacing $(\omega_{1j} \cup \omega_{2j}) \setminus \{K_+ \cup K_-\}$ by $\omega_{1j} \cup \omega_{2j}$.

We can also replace $\omega_{3j} \setminus \{K_+ \cup K_-\}$ by ω_{3j}. This enlarges the negative part, however, regions ω_{3j} exist only for the curved segments of Γ and those are by assumption inside $B_{\frac{1}{2}r_0}(O)$, while the regions $K_\pm$ are by construction outside $B_{r_0}(O)$, which implies that such an error is $\mathcal{O}(\mathrm{e}^{-3\xi r_0/2})$ and can be again neglected.

Conclusion of the proof

The estimate now contains only integrals over sectors ω_{kj} which are easy to evaluate explicitly; this proves the theorem under assumption (p3).

To complete the proof we use the following *approximation result*:

Theorem (Sabitov-Slovesnov (2010))

Let Γ be a C^3-smooth curve consisting of a finite number of segments such that on each of them the monotonicity character of the signed curvature $\kappa(\cdot)$ of Γ and its sign are preserved. Then Γ can be approximated by a C^1-smooth function $\hat\Gamma$ of the same length, the curvature of which is piecewise constant having jumps at the points $s_1 < s_2 < \cdots < s_N$, in the sense that the estimates

$$\|\Gamma^{(m)} - \hat\Gamma^{(m)}\|_\infty \le C \max_{1\le k\le N-1} (s_{k+1} - s_k)^{3-m}, \quad m = 0, 1, 2,$$

hold with some $C > 0$ for the function Γ and its two first derivatives.

It is straightforward to check that all the used estimates persist when we approximate our curve by a family of arc arrays, $\Gamma_n \to \Gamma$.

Convexity and potential bias

Theorem

Assume $V_0 \geq 0$ together with (s1)–(s3) and (p1). If one of the regions $\Omega_\pm$ is convex and (p3) holds, then $H_{\Gamma,V}$ has at least one discrete eigenvalue. If $V_0 > 0$ and Ω_+ is convex, the operator $H_{\Gamma,V}$ has at least one discrete eigenvalue provided that (p4) holds.

Note that these claims *do not need mirror symmetry* of the potential v.

The construction of the trial function proceed as in the previous case but we have to distinguish the two sides, $\Omega_\pm$, with different $\xi_\pm$; this requires the indicated stronger geometric restrictions.

In the *zero-energy resonance* situation the quadratic form is estimated by

$$Q_{V_0}[\psi] = -\frac{1}{8}\delta\nu - \int_{\mathbb{R}} \kappa(s)\,\mathrm{d}s + o(\psi),$$

where the error term can be made arbitrarily small by choosing large enough parameters r_0 and s^*; it obviously works in the *convex* case only when the integral is positive.

Many questions remain open

- Another weak-coupling problem concerns the effect of a *slight bend* for a soft guide of a constant profile. One conjectures that in analogy to the Dirichlet tubes and leaky curves the leading term would be proportional to the *fourth power of the bending angle*.

- Back to non-asymptotic problems, one may ask what happens in 3D waveguides when the profile does not have rotational symmetry and *Tang condition is violated*. It is known that in Dirichlet waveguides with *torsion* gives rise to an effective with *repulsive interaction* but for leaky and soft guides the problem may be more complicated.

T. Ekholm, H. Kovařík, D. Krejčiřík: A Hardy inequality in twisted waveguides, *Arch. Rat. Mech. Anal.* **188** (2008), 245–264.

- Potential channels of a more complicated geometry, in first place *branched ones* built over a metric graph. Of course, to have the problem well defined one must specify the potential in the vicinity of the graph vertices because the spectrum would depend on it.

More problems

- Another question concerns *scattering* in a bent or locally perturbed potential channel including possible *resonance effects* in narrow and sufficiently deep channels.
- Another extension to three dimensions concerns *potential layers*, that is potentials of a fixed transverse profile built over an infinite surface Σ in $\mathbb{R}^3$. One can again establish the discrete spectrum existence for potential layers with the profile deep enough, while in the regime different from the asymptotic one, the question is open.
- For layers the spectrum may depend on the *global* geometry of the interaction support. An example of a *conical* potential layer was found, and recently the conclusion have been extended to layers with *asymptotically cylindrical ends*.

S. Egger, J. Kerner, K. Pankrashkin: Discrete spectrum of Schrödinger operators with potentials concentrated near conical surfaces, *Lett. Math. Phys.* **110** (2020), 945–968.

D. Krejčiřík, J. Kříž: Bound states in soft quantum layers, `arXiv:2205.04919`

- and the list may continue, *ad libitum*

Closing the book

So far we have assumed that *asymptote angle is nonzero*; let us now look what happens if this angle tends to zero.

Without loss of generality we may assume that the curved part of Γ is in the *left halfplane*, while $\Gamma_\pm := \big\{ \big(x_1, \pm(\rho + x_1 \tan(\frac{1}{2}\beta)\big) : x_1 \geq 0 \big\}$ with a positive ρ and $\beta \in [0, \frac{1}{2}\pi)$ are its straight parts are, symmetric with respect to the x axis.

In addition to $h_v = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} - v(x)$ we need also the double-well operator

$$h_{v,\rho} = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} - v(\rho + x) - v(-\rho - x)$$

It is easy to see that its spectral threshold $\epsilon_{v,\rho}$ is *monotonously increasing* and converges to the spectral threshold ϵ_v of h_v as $\rho \to \infty$.

We know already that $\sigma_{\mathrm{ess}}(H_{\Gamma,\mu}) = [\epsilon_v, \infty)$ holds for any $\beta > 0$ and it is easy to see that $\sigma_{\mathrm{ess}}(H_{\Gamma,V}) = [\epsilon_{v,\rho}, \infty)$ if $\beta = 0$. It shows that the discrete spectrum of $H_{\Gamma,V}$ must *fill the gap* between $\epsilon_{v,\rho}$ and ϵ_v as $\beta \to 0$.

Spectral accumulation

We are therefore interested how the spectrum behaves in the limit $\beta \to 0$:

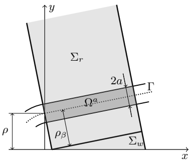
Theorem

Under the stated assumptions, there is a $C_\nu > 0$ for any $\nu \in (\epsilon_{v,\rho}, \epsilon_v)$ such that $\dim E_{H_{\Gamma,V}}(\epsilon_{v,\rho}, \nu) \geq C_\nu \beta^{-1}$ holds for the corresponding spectral projection of $H_{\Gamma,V}$ provided that β is small enough.

P.E., D. Spitzkopf: Tunneling in soft waveguides: closing a book, *J. Phys. A: Math. Theor.* **57** (2024), 125301

Proof is variational using trial functions of the form

$$\phi(x,y) := \left[\chi_{\Sigma_r}(x,y)\varphi_{\rho_\beta}(u(x,y)+\rho_\beta) + \chi_{\Sigma_w}(x,y)\varphi_{\rho_\beta}(0)\right] f(s(x,y)), \quad y \geq 0,$$



where φ_{ρ_β} is the double-well ground-state eigenfunction, $u(x,y)$ is the distance from the curve, $s(x,y)$ is the arc length coordinate on Γ, and the function $f \in C^2(\mathbb{R})$ satisfies $f(s_1) = f(s_2) = 0$

Spectral accumulation

Denoting $L = s_2 - s_1$ and $\rho_\beta = \rho \sec\frac{\beta}{2}$ we obtain by straigthforward computation the value of the shifted quadratic form of $H_{\Gamma,V}$,

$$\mathbf{q}[\phi] - \nu\|\phi\|^2 = \|f'\|^2 \Big[\|\varphi_{\rho_\beta}\|^2 + |\varphi_{\rho_\beta}(0)|^2 L \tan\tfrac{\beta}{2}\Big]$$
$$+ \|f\|^2 \Big[\big(\epsilon_{v,\rho_\beta} - \nu\big)\|\varphi_{\rho_\beta}\|^2 - \nu|\varphi_{\rho_\beta}(0)|^2 L \tan\tfrac{\beta}{2}\big)\Big]$$

which is negative provided

$$\frac{\|f'\|^2}{\|f\|^2} < \frac{\nu - \epsilon_{v,\rho_\beta} + \nu\eta_{\rho_\beta}^2 L \tan\frac{\beta}{2}}{1 + \eta_{\rho_\beta}^2 L \tan\frac{\beta}{2}}, \quad \eta_{\rho_\beta} := \frac{|\varphi_{\rho_\beta}(0)|}{\|\varphi_{\rho_\beta}\|}.$$

However, the left-hand side refers to Dirichlet Laplacian on an interval of length L, hence the maximum number n_ν of mutually orthogonal trial functions making $\mathbf{q}[\cdot] - \nu\|\cdot\|^2$ negative comes from the requirement that $\big(\frac{\pi n_\nu}{L}\big)^2$ is smaller that the right-hand side; changing L as β decreases in such a way that $L\beta = \mathrm{const}$, we get the result. $\square$

Parallel asymptotes, weak coupling

Next we ask whether $\sigma_{\rm disc}(H_{\Gamma,V}) \neq \emptyset$. The answer is *negative* if the channel-profile potential is *weak*:

Theorem

Under the stated assumptions, $\sigma_{disc}(H_{\Gamma,\lambda V})$ is empty for all λ small enough

To see that we use bracketting and add Neumman condition at the y axis splitting the curved and asymptote part of the channel,

$$H_{\Gamma,\lambda V} \geq H^{\rm c}_{\Gamma,\lambda V} \oplus H^{\rm a}_{\Gamma,\lambda V}.$$

Using separation of variables in the right halfplane, we find that

$$\inf\sigma(H_{\Gamma,\lambda V}) = \inf\sigma(H^{\rm a}_{\Gamma,\lambda V}) = \lambda^2\|v_\rho\|_1^2 + \mathcal{O}(\lambda^3) \quad \text{as} \;\; \lambda\to 0,$$

where $v_\rho(x) := v(\rho+x) + v(-\rho-x)$. On the other hand, completing the curved part by it mirror image in the right halfplane, we get

$$\epsilon_0(\lambda) = -\big(C_V + o(1)\big)\exp\Big(-\frac{2\pi}{\lambda\|V^{\rm a}\|_1}\Big) \quad \text{as} \;\; \lambda\to 0$$

Parallel asymptotes, strong coupling

There are various way to make the channel deep, e.g., by replacing the potential V by $V + \lambda\chi_{\Omega^a}$ where Ω^a is the potential support:

Theorem

Under the stated assumption, $\sigma_{\mathrm{disc}}(H_{\Gamma,V+\lambda\chi_{\Omega^a}}) \neq \emptyset$ for all λ large enough.

The claim follows from two observations: (i) the 'shifted' operator family $\{H_{\Gamma,V+\lambda\chi_{\Omega^a}} + \lambda I :\, \lambda \geq 0\}$ converges in the *generalized strong resolvent sense* to $-\Delta_{\mathrm{D}}^{\Omega^a} - V$, and (ii) the well-known result about the existence of curvature-induced bound states in Dirichlet waveguides [EK'15, Thm. 1.1] can be extended to Dirichlet channels of a *non-flat bottom*.

There are other ways the guide strongly attractive, for instance

Proposition

Let $\Gamma \in C^4(\mathbb{R})$ and consider potentials $v_{g(\lambda)}(x) := g(\lambda)v(\lambda x)$. There is a function g_0 satisfying $\lim_{\lambda\to\infty} \frac{g_0(\lambda)}{\lambda} = \infty$ as $\lambda \to \infty$ such that $\sigma_{\mathrm{disc}}(H_{\Gamma,V_{g(\lambda)}})$ is nonempty for any $g \geq g_0$ and all λ large enough.

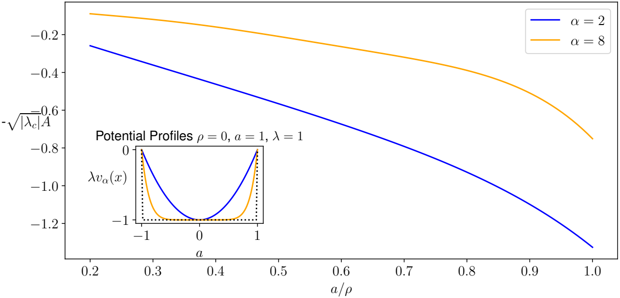
An example: critical strength

Consider an U-shaped channel with a polynomial profile given by

$$v_\alpha(x) := \min\left\{\left(\frac{|x|-\rho}{a}\right)^\alpha - 1,\ 0\right\}$$

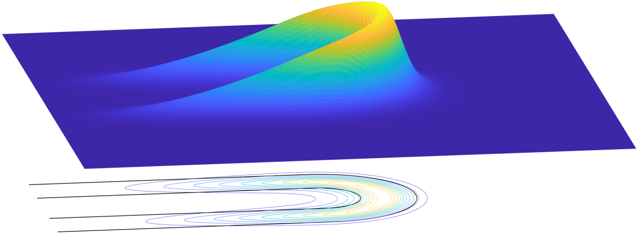
which tends to a rectangular well as $\alpha \to \infty$.

We can compute the *critical potential strength* needed to have at least one bound state, expressed through the dimensionless quantity $-\sqrt{|\lambda|}A$, where $A := \frac{1}{\pi}\int_{-a}^{a}\sqrt{v_\alpha(x)}\,\mathrm{d}x$, as a function of the ratio a/ρ



An example: ground-state eigenfunction

Using finite-element method, one can also find the eigenfunctions. As an example we plot the ground state for $\rho = 0.25$, $a = 0.1$, $\lambda = -225$ and $\alpha = 2$.



P.E., D. Spitzkopf: Tunneling in soft waveguides: closing a book, *J. Phys. A: Math. Theor.* **57** (2024), 125301

Another model: quantum dot arrays

Given a $\rho > 0$ and a *nonzero* real-valued function $V \in L^2(0, \rho)$ we define *radial potential* supported in $B_\rho(y)$ centered at $y \in \mathbb{R}^\nu$, $\nu = 2, 3$.

We consider a family of points, $Y = \{y_i\} \subset \mathbb{R}^\nu$, such that the balls $B_\rho(y_i)$ do not overlap, $\mathrm{dist}(y_i, y_j) \geq 2\rho$ if $i \neq j$, and denote $V_i : x \mapsto V(x - y_i)$. The object of our interest is the Schrödinger operator

$$H_{\lambda V, Y} = -\Delta - \lambda \sum_i V_i(x)$$

To visualise better the geometry of the system we suppose that the points of Y are distributed over a curve $\Gamma \subset \mathbb{R}^\nu$

If Y consists of a single point, we use the abbreviated symbol $H_{\lambda V}$. It is straightforward to check that $\sigma_{\mathrm{ess}}(H_{\lambda V}) = [0, \infty)$ and the discrete spectrum, written as an ascending sequence $\{\epsilon_n\}$, is at most finite.

In two dimensions it is nonempty provided $\int_0^\rho V(r)\, r\mathrm{d}r > 0$, for $\nu = 3$ the existence of bound states requires a critical interaction strength.

A straight array

Consider first the geometrically trivial case where the set $Y = Y_0$ is invariant w.r.t. discrete translations, i.e. the $\Gamma = \Gamma_0$ is a straight line:

Proposition

$\sigma(H_{V,Y_0}) \supset [0, \infty)$. *If* $\int_0^\rho V(r)\, r^\nu \mathrm{d}r > 0$, *we have* $\inf \sigma(H_{V,Y_0}) < 0$, *and the spectrum may or may not have gaps. Their number is finite and does not exceed* $\#\sigma_{\mathrm{disc}}(H_V)$. *This bound is saturated for the spacing a large enough if* $\nu = 2$, *in the case* $\nu = 3$ *there may be one gap less which happens if the potential is weak, i.e. for* $H_{\lambda V, Y_0}$ *with* λ *sufficiently small.*

- For positive energies it is easy to construct a Weyl sequence
- In the negative part by Floquet decomposition we consider a *single potential well in a slab* S^a of width a using two-sided estimates by the symmetric/antisymmetric solutions
- Negative spectrum existence is proved using a a suitable trial function
- Note that $\inf \sigma(H_{V,Y_0}) < 0$ even if a single well in 3D is *subcritical*

The essential spectrum

Suppose now that $\Gamma : \mathbb{R} \to \mathbb{R}^\nu$ is a unit-speed curve, $|\dot\Gamma| = 1$, i.e., the curve is parametrized by its arc length, and the points of the array Y_Γ are *distributed equidistantly* with respect to this variable with a spacing satisfying again $a \geq 2\rho$, as required by the potential wells disjointness.

In addition, the potential components of the operator $H_{V,Y}$ must not overlap: we assume that $|\Gamma(s+a) - \Gamma(s)| \geq 2\rho$ holds for any $s \in \mathbb{R}$.

Using Neumann bracketing, it is not difficult to prove the following claim:

Proposition

Let Γ be straight outside a compact set and let $|\Gamma(s) - \Gamma(-s)| \to \infty$ hold as $|s| \to \infty$, then $\inf \sigma_{\mathrm{ess}}(H_{V,Y})$ is the same as in the case of a straight array of the same spacing.

Birman-Schwinger principle again

Suppose now that the array potentials are *purely attractive*, $V \geq 0$. The symmetry of the potentials V allows us to use *Birman-Schwinger principle* more effectively inspectig the spectrum of the operator

$$K_{V,Y}(z) := V_Y^{1/2}(-\Delta - z)^{-1} V_Y^{1/2}, \quad V_Y := \sum_i V_i.$$

Note that since the supports of the V_i's are disjoint, we can write $K_{V,Y}$ in the 'matrix' form with the 'entries' $K_{V,Y}^{(i,j)}(-\kappa^2) := V_i^{1/2}(-\Delta + \kappa^2)^{-1} V_j^{1/2}$.

The crucial part of the argument is the following equivalence:

Proposition

$z \in \sigma_{\mathrm{disc}}(H_{V,Y})$ *holds if and only if* $1 \in \sigma_{\mathrm{disc}}(K_{V,Y}(z))$ *and the dimensions of the corresponding eigenspaces coincide. The operator* $K_{V,Y}(-\kappa^2)$ *is bounded for any* $\kappa > 0$ *and the function* $\kappa \mapsto K_{V,Y}(-\kappa^2)$ *is continuously decreasing in* $(0,\infty)$ *with* $\lim_{\kappa\to\infty} \|K_{V,Y}(-\kappa^2)\| = 0$.

Curvature-induced bound states

Theorem

Suppose that $\Gamma \neq \Gamma_0$ satisfy the stated assumptions and $V \geq 0$, then $\inf \sigma(H_{V,Y}) < \epsilon_0 := \inf \sigma_{\text{ess}}(H_{V,Y})$*, and consequently,* $\sigma_{\text{disc}}(H_{V,Y}) \neq \emptyset$.

P.E.: Geometry effects in quantum dot families, *Pure Appl. Funct. Anal.*, to appear; arXiv:2305.12748

Sketch of the proof: We have to show that there is a $\kappa > \sqrt{-\epsilon_0}$ such that $K_{V,Y}(-\kappa^2)$ has eigenvalue one. Due to the mentioned monotonicity of the BS operator with respect to κ, it is sufficient to check that

$$\sup \sigma(K_{V,Y}(-\kappa^2)) > \epsilon_{\text{ess}}(\kappa) := \sup \sigma_{\text{ess}}(K_{V,Y}(-\kappa^2)$$

holds for any $\kappa > 0$. To this aim, we construct a trial function ψ such that

$$(\phi, K_{V,Y}(-\kappa_0^2)\phi) - \|\phi\|^2 > 0$$

where the first expression can be rewritten explicitly as

$$\sum_{i,j\in\mathbb{Z}} \int_{B_\rho(y_i)\times B_\rho(y_j)} \overline{\phi}(x) V_i^{1/2}(x)(-\Delta + \kappa_0^2)^{-1}(x,x') V_j^{1/2}(x')\phi(x')\,\mathrm{d}x\,\mathrm{d}x'.$$

Trial function

Denote by ϕ_0 the *generalized eigenfunction* of $K_{V,Y}(-\kappa_0^2)$ referring to $\inf\sigma(H_{V,Y_0})$; as the product of the corresponding *gef* of H_{V,Y_0} and $V_Y^{1/2}$, it is *periodic* and we regard it as *real-valued* and *positive*.

The restrictions $\phi_{0,i} = \phi_0 \upharpoonright B_\rho(y_i)$ are copies of the same function properly shifted, $\phi_{0,i}(\xi) = \phi_0(\xi + y_i)$ for $\xi \in B_\rho(0)$. The symmetries of ϕ_0 imply, in particular, that $\phi_{0,i}(-\xi) = \phi_{0,i}(\xi)$ holds for $\xi \in B_\rho(0)$.

For a given Y the functions ϕ_0^Y as an *'array of beads'*: its values in $B_\rho(y_i)$ would coincide with $\phi_{0,i}$ the axis of which is *aligned with the tangent* to Γ at the point y_i. To make such a function an L^2 element, we need a suitable family of mollifiers; we choose it in the form

$$h_n(x) = \frac{1}{2n+1}\,\chi_{M_n}(x), \quad n \in \mathbb{N}.$$

where $M_n := \{x :\ \mathrm{dist}(x, \Gamma \upharpoonright [-(2n+1)a/2, (2n+1)a/2]) \le \rho\}$ is a 2ρ-wide closed tubular neighborhood of the $(2n+1)a$-long arc of Γ.

The inequality to be checked

The influence of such a cut-off can be made arbitrarily small:

Lemma

$(h_n\phi_0^Y, K_{V,Y}(-\kappa_0^2)h_n\phi_0^Y) - \|h_n\phi_0^Y\|^2 = \mathcal{O}(n^{-1})$ as $n\to\infty$.

Consequently, it is sufficient to check that

$$\lim_{n\to\infty}(h_n\phi_0^Y, K_{V,Y}(-\kappa_0^2)h_n\phi_0^Y) - (h_n\phi_0 K_{V,Y_0}(-\kappa_0^2)]h_n\phi_0) > 0,$$

or – with an abuse of notation neglecting the rotation of $\phi_{0,i}$ – that

$$(\phi_0, [K_{V,Y}^{(i,j)}(-\kappa^2) - K_{V,Y_0}^{(i,j)}(-\kappa^2)]\phi_0) \geq 0$$

holds any $\kappa > 0$ and all $i,j \in \mathbb{Z}$ being *positive* for some of them.

If $Y \neq Y_0$, however, there is a pair of indices for which this is not the case, $|y_i - y_j| < |i-j|a$, in fact, infinitely many such pairs. The *monotonicity* of the resolvent kernel is *not sufficient*, though, because bending of the chain may cause some distances between points of potential supports outside the ball centers to *increase*.

Convexity enters the game

Denoting the resolvent kernel by $G_{i\kappa}$, we can rewrite the expression as

$$\int_{B_\rho(0)}\int_{B_\rho(0)} \phi_0(\xi)V^{1/2}(\xi)\big[G_{i\kappa}(y_i-y_j+\xi-\xi')-G_{i\kappa}(y_i^{(0)}-y_j^{(0)}+\xi-\xi')\big]$$

$$\times V^{1/2}(\xi')\phi_0(\xi')\mathrm{d}\xi\,\mathrm{d}\xi'$$

$$=\frac{1}{2}\int_{B_\rho(0)}\int_{B_\rho(0)} \phi_0(\xi)V^{1/2}(\xi)\big[G_{i\kappa}(y_i-y_j+\xi-\xi')-G_{i\kappa}(y_i^{(0)}-y_j^{(0)}+\xi-\xi')$$

$$+G_{i\kappa}(y_i-y_j-\xi+\xi')-G_{i\kappa}(y_i^{(0)}-y_j^{(0)}-\xi+\xi')\big]V^{1/2}(\xi')\phi_0(\xi')\mathrm{d}\xi\,\mathrm{d}\xi,$$

where we used the symmetry, $\phi_0(\xi)V^{1/2}(\xi)=\phi_0(-\xi)V^{1/2}(-\xi)$.

The integration over ξ can be split by orientation with respect to y_i-y_j, specifically, we have $\int_{B_\rho(0)}\mathrm{d}\xi=\int_{-\rho}^{\rho}\mathrm{d}\xi_\perp\int_{-\sqrt{\rho^2-s_\perp^2}}^{\sqrt{\rho^2-s_\perp^2}}\mathrm{d}\xi_{||}$.

Now not only the function $G_{i\kappa}(\cdot)$ is *convex*, but the same is true for $G_{i\kappa}(|y_i-y_j|+\cdot)-G_{i\kappa}(|y_i^{(0)}-y_j^{(0)}|+\cdot)$ as long as $|y_i-y_j|<|y_i^{(0)}-y_j^{(0)}|$, hence *Jensen's inequality* yields

$$G_{i\kappa}(|y_i-y_j|)-G_{i\kappa}(|y_i^{(0)}-y_j^{(0)}|)>0.$$

Proof conclusion and comments

In combination with the positivity of $\phi_0 V^{1/2}$ this proves that the right-hand side is *positive* whenever $|y_i - y_j| < |i-j|a$; this in turn concludes the proof.

Note the role of the symmetry of V. Without is, the deformation of Γ had to be strong enough to diminish *all* the distances between the points of the pairs of balls; this is true, e.g., if $|y_i - y_{i+1}| < a - 2\rho$ holds for neighboring balls, which is clearly far from optimal.

One the other hand, *shrinking* the potential wells using an appropriate *nonlinear scaling* one can *approximate point interactions*, which requires neither symmetry of V not it positivity.

S. Albeverio, F. Gesztesy, R. Høegh-Krohn, H. Holden: Solvable Models in Quantum Mechanics, 2nd edition, Amer. Math. Soc., Providence, R.I., 2005.

For the limiting operator the analogous result is known: an infinite 'locally equidistant' array of point interactions in dimension $\nu = 2, 3$ which not straight, but is asymptotically straight has a *nonempty discrete spectrum*.

P.E.: Bound states of infinite curved polymer chains, *Lett. Math. Phys.* **57** (2001), 87–96.

This suggests that our result is likely to hold under weaker assumptions.

Finite soft guides: an optimization

The question we have in mind concerns the *spectral optimization* in analogy with what is known in Dirichlet and δ potential cases

P.E., E.M. Harrell, M. Loss: Optimal eigenvalues for some Laplacians and Schrödinger operators depending on curvature, in *Mathematical Results in Quantum Mechanics*, Birkhäuser, Basel 1999; pp. 47–53.

P.E., E.M. Harrell, M. Loss: Inequalities for means of chords, with application to isoperimetric problems, *Lett. Math. Phys.* **75** (2006), 225–233; addendum **77** (2006), 219.

Let Γ be a C^2-smooth *loop* without self-intersections of a *fixed length L*. For small enough positive $d_\pm$ the map $[0, L) \times \mathcal{J} \ni (s, u) \mapsto \Gamma(s) + u\nu(s)$, where $\mathcal{J} = [-d_-, d_+]$ and $\nu = (-\dot\Gamma_2, \dot\Gamma_1)$ is the normal to Γ, is *bijective*.

We consider operators $H_{\gamma,\mu}$ corresponding the measure-type interaction

$$\mu(M) := \int_0^L \int_{-d_-}^{d_+} \chi_M\big(\Gamma(s) + u\nu(s)\big)\,(1 + u\gamma(s))\,\mathrm{d}\mu_\perp(t)\mathrm{d}s,$$

where the positive transverse measure $\mu_\perp$ can describe both a regular attractive potential channel we are discussing here, $\mu_\perp(u) = V(u)\mathrm{d}u$, as well as a δ potential, and more.

Ground state optimization

We define $H_{\Gamma,\mu}$ as the self-adjoint operator associated with the form

$$h_{\Gamma,\mu}[\psi] := \|\nabla\psi\|^2 - \int_{\mathbb{R}^2} |\psi|^2 \mathrm{d}\mu, \quad \mathrm{dom}\, h_{\Gamma,\mu} = H^1(\mathbb{R}^2).$$

It is not difficult to check that the essential spectrum of $H_{\Gamma,\mu}$ is $[0,\infty)$ and $\sigma_{\mathrm{disc}}(H_{\Gamma,\mu}) \neq \emptyset$. Let $\mathcal{C}$ be a *circle of radius* $\frac{L}{2\pi}$. By $\mu_\circ$ we denote the corresponding measure generated by $\mu_\perp$ and giving rise to operator $H_{\Gamma,\mu_\circ}$.

Theorem

The lowest eigenvalues $\lambda_1(\mu)$ and $\lambda_1(\mu_\circ)$, respectively, of $H_{\Gamma,\mu}$ and of $H_{\Gamma,\mu_\circ}$ satisfy the inequality

$$\lambda_1(\mu) \leq \lambda_1(\mu_\circ).$$

We *conjecture* that the inequality is strict unless Γ and $\mathcal{C}$ are congruent.

Note also that this provides an *alternative proof* of the leaky loop result.

Ground state optimization

The claim follows by a simple *variational argument*: the appropriate trial function is obtained using the lowest eigenfunction of $H_{\Gamma,\mu_\circ}$ and *'transplanting'* it to the parallel coordinates.

More specifically, we take trial functions ψ the values which, inside and outside the loop, are of the form $u(\mathrm{dist}(x,\Gamma))$ where u is a C_0^∞ function. Using appropriate changes of the variables, we check that the inequality $h_{\Gamma,\mu}[\psi] \le h_{\mathcal{C},\mu}[\psi]$ holds for any such u; comparing then the Rayleigh quotients we arrive at the result. It has a slight generalization:

Theorem

Let χ, respectively $\chi_\circ$, be the indicator function of the open set inside the loop strip. The lowest spectral points $\lambda_1^\beta(\mu)$ and $\lambda_1^\beta(\mu_\circ)$ of $H_{\Gamma,\mu} + \beta\chi$ and $H_{\Gamma,\mu_\circ} + \beta\chi_\circ$, respectively, satisfy then the inequality

$$\lambda_1^\beta(\mu) \le \lambda_1^\beta(\mu_\circ).$$

In particular, $\sigma_{\mathrm{disc}}(H_{\Gamma,\mu_\circ} + \beta\chi_\circ) \neq \emptyset$ implies $\sigma_{\mathrm{disc}}(H_{\Gamma,\mu} + \beta\chi) \neq \emptyset$.

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

Another optimization result

One can also optimize with respect to the *channel profile*:

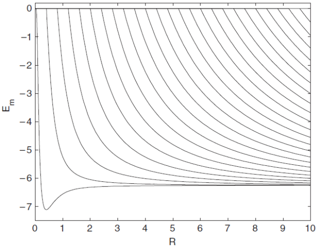
Theorem

Put $\alpha := \mu_\perp(\mathcal{J})$ *and consider Schrödinger operators* $H_{\Gamma_t,\alpha}$, *where* Γ_t *is 'parallel' to* Γ *at the distance* t, *then the lowest eigenvalues* $\lambda_1(\mu)$ *and* $\lambda_1(\alpha\Gamma_t)$ *of* $H_{\Gamma,\mu}$ *and of* $H_{\Gamma_t,\alpha}$, *respectively, satisfy the inequality*

$$\lambda_1(\mu) \geq \min_{u\in\mathcal{J}} \lambda_1(\alpha\Gamma_t).$$

This is again easy to prove variationally; one has to check that the function $\mathcal{J} \ni t \mapsto \|\psi|_{\Gamma_t}\|^2$ is continuous so that it attains its maximum value at some $t_\star = t_\star(\mu) \in \mathcal{J}$.

Depending on α, the position of $t_\star$ in $\mathcal{J}$ may be at different; recall how the eigenvalues $H_{\mathcal{C},\alpha}$, here with $\alpha = 5$, depend on the circle radius



Optimization for finite dot arrays

Consider the 2D situation and fix the curve Γ as a *circle* of radius R on which we place centers of the disks $B_\rho(y_i)$; without loss of generality we place the circle center to the origin of the coordinates. The support balls again do not overlap, $\rho \le R \sin \frac{\pi}{N}$, where $N := \#Y$.

It is again the maximum-symmetry configuration which maximizes the principal eigenvalue of $H_{V,Y}$:

Theorem

Up to rotations, $\epsilon_1(H_{V,Y}) := \inf \sigma(H_{V,Y})$ is uniquely maximized by the configurations in which all the neighboring points of Y have the same angular distance $\frac{2\pi}{N}$.

Proof sketch: The negative spectrum of $H_{V,Y}$ is now discrete and finite, and $\epsilon_1(H_{V,Y})$ is a simple eigenvalue. We denote by Y_{sym} the symmetric array. The real-valued eigenfunction ψ_{sym} associated with $\epsilon_1(H_{V,Y_{\mathrm{sym}}})$ has the appropriate symmetry: in polar coordinates we can express it as $\psi_{\mathrm{sym}}(r,\varphi) = \psi_{\mathrm{sym}}(r,\varphi + \frac{2\pi n}{N})$ for any $n \in \mathbb{Z}$.

Optimization for finite dot arrays

We use BS principle again and denote by $\phi_{\rm sym}$ the eigenfunction corresponding to the *largest eigenvalue* of $K_{V,Y_{\rm sym}}(\epsilon_{\rm sym})$, where $\epsilon_{\rm sym} = \inf\sigma(H_{V,Y_{\rm sym}})$.

It has the same symmetry and may be again regarded as real-valued and positive. In analogy with the previous proof we are looking for a trial function ϕ_Y such that

$$(\phi_Y, K_{V,Y}(-\kappa_0^2)\phi_Y) - \|\phi_Y\|^2 > 0, \quad \kappa_0 = \sqrt{-\epsilon_{\rm sym}}.$$

As before ϕ_Y will be an *'array of beads'*; we take $\phi_{\rm sym} \upharpoonright B_\rho(y_1)$ calling it $\phi_{{\rm sym},1}$ and use it to create $\phi_{{\rm sym},j}$, $j = 2,\dots,N$, by rotating this function on the angle $\sum_{i=1}^{j-1}\theta_i$ around the origin. For $Y = Y_0$ the left-hand side of the inequality vanishes by construction, hence it is sufficient to prove that

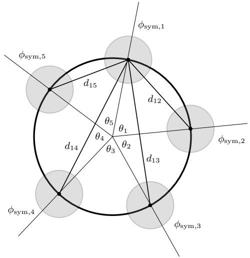
$$(\phi_Y, K_{V,Y}(-\kappa^2)\phi_Y) - (\phi_{\rm sym}, K_{V,Y_0}(-\kappa^2)\phi_{\rm sym}) > 0$$

holds for any $\kappa > 0$, in particular, for $\kappa = \kappa_0$, or explicitly

Optimization for finite dot arrays

$$\frac{1}{2\pi}\sum_{i,j=1}^{N}\Big\{\int_{B_\rho(0)}\int_{B_\rho(0)}\phi_{\rm sym}(\xi)V^{1/2}(\xi)\,K_0(\kappa|y_i+\xi-y_j-\xi'|)$$
$$\times V^{1/2}(\xi')\phi_{\rm sym}(\xi')\,\mathrm{d}\xi\,\mathrm{d}\xi'$$
$$-\int_{B_\rho(0)}\int_{B_\rho(0)}\phi_{\rm sym}(\xi)V^{1/2}(\xi)\,K_0(\kappa|y_i^{(0)}+\xi-y_j^{(0)}-\xi'|)$$
$$\times V^{1/2}(\xi')\phi_{\rm sym}(\xi')\,\mathrm{d}\xi\,\mathrm{d}\xi'\Big\}>0$$

We denote $d_{ij}:=|y_i-y_j|$ and $d_{ij}^{(0)}:=|y_i^{(0)}-y_j^{(0)}|$ as indicated in the figure,



and write the first part of the above expression as $\sum_{i,j=1}^{N}\tilde G_{i\kappa}(d_{ij})$.

Convexity again

Using this notation, the sought inequality takes the form

$$\sum_{i,j=1}^{N} \tilde{G}_{i\kappa}(d_{ij}) > \sum_{i,j=1}^{N} \tilde{G}_{i\kappa}(d_{ij}^{(0)}),$$

and rearranging the summation order, we have to check that

$$F(d_{ij}) := \sum_{m=1}^{[N/2]} \sum_{|i-j|=m} \left[\tilde{G}_{i\kappa}(d_{ij}) - \tilde{G}_{i\kappa}\big(d_{ij}^{(0)}\big)\right] > 0$$

holds for every family $\{d_{ij}\}$ which is *not congruent* with $\{d_{ij}^{(0)}\}$.

The *composed map* $d_{ij} \mapsto K_0(\kappa|y_i + \xi - y_j - \xi'|)$ is easily seen to be convex for any $\xi, \xi' \in B_\rho(0)$, and the property persists at integration with a positive weight, hence by Jensen's inequality

$$F(d_{ij}) \geq \sum_{m=1}^{[N/2]} \nu_n \Big[\tilde{G}_{i\kappa}\Big(\frac{1}{\nu_n} \sum_{|i-j|=m} d_{ij}\Big) - \tilde{G}_{i\kappa}\big(d_{i,i+m}^{(0)}\big)\Big],$$

where $\nu_n = N$ except for N even and $m = \frac{1}{2}N$, in which case $\nu_n = \frac{1}{2}N$.

Proof conclusion

It remains to use the *monotonicity* of the resolvent kernel, and thus of $\tilde{G}_{i\kappa}(\cdot)$; since $d_{ij} \mapsto |y_i + \xi - y_j - \xi'|$ is increasing, it is only necessary to check that

$$\frac{1}{\nu_n} \sum_{|i-j|=m} d_{ij} < d^{(0)}_{i,i+m}$$

for any fixed i. Denoting $\beta_{ij} = \sum_{k=i}^{j-1} \theta_k$, we have $d_{ij} = 2\sin\frac{1}{2}\beta_{ij}$ and $d^{(0)}_{i,i+m} = 2\sin\frac{\pi m}{N}$, and since the sine function is *strictly concave* in $(0,\pi)$, Jensen's inequality gives

$$\frac{1}{\nu_n} \sum_{|i-j|=m} 2\sin\frac{1}{2}\beta_{ij} < 2\sin\left(\frac{1}{\nu_n} \sum_{|i-j|=m} \frac{1}{2}\beta_{ij}\right) = 2\sin\frac{\pi m}{N} = d^{(0)}_{i,i+m}$$

for those families $\{d_{ij}\}$ of circle chords which are *not congruent* with $\{d^{(0)}_{ij}\}$; this concludes the proof.

Remarks

- By an easy modification with a *planar* circle, one can prove the analogous claim for a quantum-dot 'necklace' in *three dimensions*
- We *conjecture* that the claim extends to a wider class of functions: if points of Y are on a loop Γ of a fixed length in $\mathbb{R}^\nu$, $\nu = 2, 3$, *equidistantly in arc length*, and the balls $B_\rho(y_i)$ do not overlap, $\epsilon_1(H_{V,Y}) = \inf \sigma(H_{V,Y})$ is maximized, uniquely up to Euclidean transformations, by a *planar regular polygon* of $\#Y$ vertices.
- Optimizing a distribution on a *sphere* is much harder reminding the *Thomson problem*. We *conjecture* that if balls $B_\rho(y_i)$ centered at a sphere do not overlap, $\epsilon_1(H_{V,Y})$ is *maximized*, uniquely up to Euclidean transformations, by the following five configurations:
  - three *simplices*, with $N = 2$ (a pair antipodal points), $N = 3$ (equilateral triangle), and $N = 4$ (tetrahedron),
  - *octahedron* with $N = 6$,
  - *icosahedron* with $N = 12$.

  Note that both conjectures have proved point-interaction counterparts

  P.E.: An optimization problem for finite point interaction families, *J. Phys.: Math. Theor.* **52** (2019), 405302
- One can also consider the *minimization problem* in this context

It remains to say

Thank you for your attention!