



# Constrained quantum dynamics

**Pavel Exner**

*Doppler Institute*

*for Mathematical Physics and Applied Mathematics  
Prague*

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# Spectrum vs. parameter values and geometry



We have encountered many situations when Hamiltonians governing a guided dynamics had a discrete spectrum. We discussed mostly its *existence* and sometimes also *cardinality*, now we are going to take a closer look at the dependence of the eigenvalues on the *parameters* involved and the problem *geometry* addressing the following questions:

- The discussion of *leaky structures* in the previous lecture suggests that their spectral properties depend on the strength of the attractive singular interaction. We have seen, for instance, that *weak coupling* depends on the dimension of the system.
- It is even more important to analyze the opposite extremum, the *asymptotic behavior* in the *strong-coupling regime*,  $\alpha \rightarrow \infty$ .
- Another question concerns the asymptotic behavior in the situation when the geometric perturbation of the 'trivial' system is *gentle*.
- A trademark topic of *spectral geometry* are relations between the *spectrum* and the related *shape*; in the present context we find a number of such problems.

# Strong $\delta$ interaction asymptotics



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

Let us start with the simplest situation of a curve in the plane, avoiding first various ‘dangerous’ situations that may occur, specifically *angles*, *cusps*, *self-intersections*, and *ends*. Then we have the following result:

## Theorem

Let  $\Gamma$  be a  $C^4$  smooth curve in  $\mathbb{R}^2$  without ends, either a closed loop or infinite, asymptotically straight and without ‘near crossings’. In the limit  $\alpha \rightarrow \infty$  the  $j$ th eigenvalue of  $H_{\alpha,\Gamma}$  behaves as

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

where  $\mu_j$  is the  $j$ th eigenvalue of  $S_\Gamma = -\frac{d^2}{ds^2} - \frac{1}{4}\kappa(s)^2$  on  $L^2(0, |\Gamma|)$  or  $L^2(\mathbb{R})$ , respectively, where  $\kappa$  is curvature of  $\Gamma$ .



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

# Strong $\delta$ interaction asymptotics



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

Furthermore, if curve  $\Gamma$  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  $j$ th eigenvalue is

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

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



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

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



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 $\delta$ interaction asymptotics



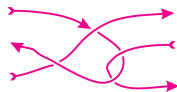
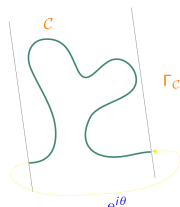
- For a *surface in  $\mathbb{R}^3$*  we replace the above  $S$  by  $S_\Gamma = -\Delta_\Gamma + K - M^2$ , where  $-\Delta_\Gamma$  is Laplace-Beltrami operator on  $\Gamma$  and  $K, M$ , respectively, are the corresponding *Gauss* and *mean* curvatures.



P.E., S. Kondej: Bound states due to a strong  $\delta$  interaction supported by a curved surface, *J. Phys. A: Math. Gen.* **36** (2003), 443-457.

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

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  $\Gamma$  be a  $C^4$ -smooth  $r$ -periodic manifold without boundary. The strong coupling asymptotic behavior of the  $j$ th Bloch eigenvalue is

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

for  $\text{codim } \Gamma = 1$  and

$$\lambda_j(\alpha, \theta) = \epsilon_\alpha + \mu_j(\theta) + \mathcal{O}(e^{\pi\alpha}) \quad \text{as } \alpha \rightarrow -\infty$$

for  $\text{codim } \Gamma = 2$ , where  $\mu_j(\theta)$  is the  $j$ th eigenvalue of the appropriate comparison operator indicated above with Bloch boundary conditions. The error terms are uniform w.r.t.  $\theta$ .



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.

## Corollary

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

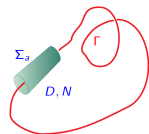


K. Yoshitomi: Band gap of the spectrum in periodically curved quantum waveguides, *J. Diff. Eqs* **142** (1998), 123-166.

## Strong $\delta$ interactions: sketch of the argument



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



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*.

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

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

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

# Strong $\delta$ interactions: sketch of the argument



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

$$t_{a,\alpha}^+[f] = \int_{-a}^a |f'(u)|^2 du - \alpha |f(0)|^2$$

and  $t_{a,\alpha}^-[f] = t_{a,\alpha}^+[f] - \|k\|_\infty (|f(a)|^2 + |f(-a)|^2)$  defined on the Sobolev spaces  $W_0^{1,2}(-a, a)$  and  $W^{1,2}(-a, a)$ , respectively. For large  $\alpha$  the presence of the boundaries cause an exponentially small error:

## Lemma

There is a positive  $c_N$  such that  $T_{\alpha,a}^\pm$  has for  $\alpha$  large enough a *single negative eigenvalue*  $\kappa_{\alpha,a}^\pm$  satisfying

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

Finally, we relate  $a$  to  $\alpha$  by choosing  $a = 6\alpha^{-1} \ln \alpha$  which yields the result. In the other cases the proof is analogous. If  $\text{codim } \Gamma = 2$  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  $\alpha \rightarrow -\infty$ .



# Curves with ends



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

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

## Theorem (E-Pankrashkin'14)

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

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

where  $\mu_j$  is the  $j$ th eigenvalue of the operator  $-\frac{d^2}{ds^2} - \frac{1}{4}\kappa(s)^2$  on  $L^2(0, L)$  with *Dirichlet b.c.*, where  $\kappa(s)$  is as before the signed curvature of  $\Gamma$  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.

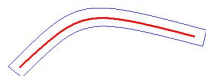
## Curves with ends: sketch of the argument



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  $\Gamma$  has by assumption *regular ends*, meaning that it can be extended smoothly in the vicinity of its endpoints.

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

We choose an *'extended' tubular neighborhood*, at each endpoint longer by  $a := \frac{6}{\alpha} \ln \alpha$ . Now we *lose 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, $\text{codim } \Gamma = 2$



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.

(i) The cardinality of the discrete spectrum behaves asymptotically as

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

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

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

where  $\mu_j$  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  $\Gamma$  can be *extended* through the boundary, in other words, that there exists a larger  $C^4$ -smooth surface  $\Gamma_2$  such that  $\bar{\Gamma} \subset \Gamma_2$ .

We consider again the comparison operator  $S_\Gamma = -\Delta_\Gamma^D + K - M^2$ , where  $-\Delta_\Gamma^D$  is Laplace-Beltrami operator on  $\Gamma$ , now with *Dirichlet condition* at  $\partial\Gamma$ , and  $K, M$ , respectively, are the *Gauss* and *mean* curvatures of  $\Gamma$ . We denote eigenvalues of this operator as  $\mu_j^D$ ,  $j \in \mathbb{N}$ , then we have

## Theorem

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

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

If, in addition,  $\Gamma$  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  $\delta$ -interactions supported by surfaces with boundaries*, *Asympt. Anal.* **97** (2016), 1–25.

## Another asymptotics: slightly bent curves



Let us turn to the other asymptotic problem mentioned in the opening. The simplest example is a *broken line*  $\Gamma = \Gamma_\beta$  with a small angle  $\beta$ .



We keep  $\alpha$  fixed and denote  $H_{\Gamma_\beta} := H_{\alpha, \Gamma_\beta}$ . We know that this operator has eigenvalues, a single one for small  $\beta$ .

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

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

holds with some constant  $a < 0$  as  $\beta \rightarrow 0+$ .

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:  $\Gamma$  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  $\Gamma : \mathbb{R} \rightarrow \mathbb{R}^2$  such that  $|\dot{\Gamma}(s)| = 1$ . Moreover,

- there exists a  $c \in (0, 1)$  such that  $|\Gamma(s) - \Gamma(s')| \geq c|s - s'|$  holds for  $s, s' \in \mathbb{R}$  excluding, in particular, *U shapes*.
- there are real numbers  $s_1 > s_2$  and straight lines  $\Sigma_i$ ,  $i = 1, 2$ , such that  $\Gamma$  *coincides with  $\Sigma_1$*  for  $s \leq s_1$  and *with  $\Sigma_2$*  for  $s \geq s_2$ ,
- *one-sided limits* of  $\dot{\Gamma}$  *exist* at the points where the function  $\ddot{\Gamma}$  is discontinuous, i.e.  $\Gamma$  has *angles* there.

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  $\Pi = \{p_i\}_{i=1}^{\#\Pi}$  and shall speak of them as of *vertices*. Consequently,  $\Gamma$  consists of  $\#\Pi + 1$  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

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

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

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  $\gamma, \tilde{\gamma}$  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*.

One can reconstruct  $\Gamma$  from  $\tilde{\gamma}$ , uniquely up to Euclidean transformations,

$$\Gamma(s) = \left( \int_0^s \cos \phi(u, 0) du, \int_0^s \sin \phi(u, 0) du \right).$$

## Weakly bent curves, continued



Now we introduce the one-parameter family of *'scaled' curves*  $\Gamma_\beta$ ,

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

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

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

$$\mathcal{A}(s, s') := \frac{\alpha^4}{32\pi} K'_0 \left( \frac{\alpha}{2} |s - s'| \right) \left( |s - s'|^{-1} \left( \int_{s'}^s \phi(s'') ds'' \right)^2 - \int_{s'}^s \phi(s'')^2 ds'' \right).$$

### Lemma

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



# 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  $H_{\Gamma_\beta}$  has a **unique eigenvalue**  $\lambda(H_{\Gamma_\beta})$  which admits the asymptotic expansion

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



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

Proof is again based on the generalized Birman-Schwinger principle which we recall here: it says that

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

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

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

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

## Weakly bent curves, continued



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

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

$$\mathcal{A}(s, s') = \frac{\alpha^4}{32\pi} K'_0\left(\frac{\alpha}{2}|s-s'|\right) \frac{|ss'|}{|s-s'|} \chi_\Omega(s, s'),$$

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

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



We can pose the same question in dimension three but it is more subtle, because then *global properties* of the interaction support play now role; recall that a conical surface, however 'flat' it may be, i.e. for any  $\theta > 0$ , gives rise to an *infinite discrete spectrum*

Let us thus restrict our attention to *locally deformed planes*: consider  $\Gamma = \Gamma_\beta(f) \subset \mathbb{R}^3$  with  $\beta > 0$  given by

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

where  $f: \mathbb{R}^2 \rightarrow \mathbb{R}$  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  $\beta \rightarrow 0+$ .

# The asymptotic expansion



The method to use is again Birman-Schwinger analysis; it yields

## Theorem

Let  $\alpha > 0$  be fixed and set

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

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

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



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

# Spectral optimization



Let us turn to the other topic mentioned in the opening. A traditional spectral geometry question is about the *shape* which makes a given property *optimal*.

Quite often the optimal shape has a *symmetry*; the most classical example is the *Faber-Krahn inequality* proving a conjecture put forward by *Lord Rayleigh*: let  $\lambda_1(\Omega)$  be the principal eigenvalues of the *Dirichlet Laplacian*  $-\Delta_{\Omega}^D$  for a region  $\Omega \subset \mathbb{R}^d$ . Assuming that  $\text{vol}(\Omega)$  is *kept fixed*, then  $\lambda_1(\Omega)$  is *sharply minimized* by a *ball*.



G. Faber: Beweis dass unter allen homogenen Membranen von gleicher Fläche und gleicher Spannung die kreisförmige den Tiefsten Grundton gibt, *Sitzungber. der math.-phys. Klasse der Bayerische Akad. der Wiss. zu München* (1923), 169–172.



E. Krahn: Über eine von Rayleigh formulierte minimal Eigenschaft des Kreises, *Ann. Math.* **94** (1925), 97–100.

To give one more example, let us mention the *Payne-Pólya-Weinberger inequality*: in the same situation the *ratio* of the first two eigenvalues,  $\frac{\lambda_2(\Omega)}{\lambda_1(\Omega)}$ , is sharply *maximized* by a ball.

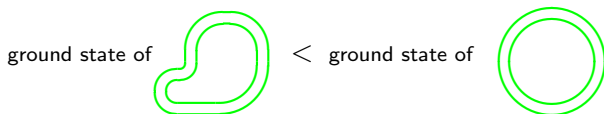


M.S. Ashbaugh, R.D. Benguria: A sharp bound for the ratio of the first two eigenvalues of Dirichlet Laplacians and extensions, *Ann. Math.* **135** (1992), 601–628.

# Non-simply connected regions



Not always does the intuition tells us the right answer. For instance, the *topology may play role*. Let us mention pictorially two examples in maximum symmetry may lead to *maximum* of the principal eigenvalue. If we seek extremum among *strips of fixed length and width* we have

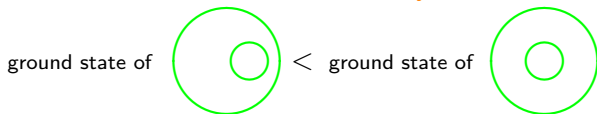


whenever the strip is not a circular annulus.



P.E., E.M. Harrell, M. Loss: Optimal eigenvalues for some Laplacians and Schrödinger operators depending on curvature, in *Proceedings of QMath7*, Birkhäuser, Basel 1999; pp. 47–53.

Similarly, for a *circular obstacle in circular cavity* we have



whenever the obstacle is off center; the minimum is reached when it is touching the boundary.



E.M. Harrell, P. Kröger, K. Kurata: On the placement of an obstacle or a well so as to optimize the fundamental eigenvalue, *SIAM J. Math. Anal.* **33** (2001), 240–259.

# A leaky loop analogue



Let  $\Gamma$  be a *loop* in  $\mathbb{R}^d$ ,  $d \geq 2$ , parametrized by its arc length, i.e. a *piecewise differentiable* function  $\Gamma : [0, L] \rightarrow \mathbb{R}^d$  such that  $\Gamma(0) = \Gamma(L)$  and  $|\dot{\Gamma}(s)| = 1$  for all but finitely many  $s \in [0, L]$ . We have

## Theorem

Let  $d = 2$ . For any  $\alpha > 0$  and  $L > 0$  we have  $\lambda_1(\alpha, \Gamma) \leq \lambda_1(\alpha, \mathcal{C})$ , where  $\mathcal{C}$  is a *circle of perimeter  $L$* , the inequality being *sharp* unless  $\Gamma$  is congruent with  $\mathcal{C}$ .



P.E., E.M. Harrell, M. Loss: Inequalities for means of chords, with application to isoperimetric problems, *Lett. Math. Phys.* **75** (2006), 242–233; addendum **77** (2006), 219.

One more time, we employ the generalized *Birman-Schwinger principle* by which there is one-to-one correspondence between eigenvalues  $-\kappa^2$  of  $H_{\alpha, \Gamma}$  and solutions to the integral-operator equation

$$\mathcal{R}_{\alpha, \Gamma}^{\kappa} \phi = \phi, \quad \text{where } \mathcal{R}_{\alpha, \Gamma}^{\kappa}(s, s') := \frac{\alpha}{2\pi} K_0(\kappa |\Gamma(s) - \Gamma(s')|)$$

on  $L^2([0, L])$ , where  $K_0$  is the Macdonald function.

# Rephrasing it as a geometric problem



We employ *inequalities on mean values of chords* denoted as  $C_L^p(u)$ :

$$\int_0^L |\Gamma(s+u) - \Gamma(s)|^p ds \leq \frac{L^{1+p}}{\pi^p} \sin^p \frac{\pi u}{L}, \quad p > 0, \quad u \in (0, \frac{1}{2}L]$$

This *may not be true for all*  $p > 0$ , however, a simple Fourier analysis allows one to demonstrate the following result:

## Proposition

$C_L^2(u)$  is valid for any  $u \in (0, \frac{1}{2}L]$ , and the inequality is strict unless  $\Gamma$  is a planar circle; by convexity the same is true for all  $p < 2$ .

Using a variational argument together with the fact that  $K_0(\cdot)$  appearing in the resolvent kernel is *strictly monotonous and convex* the optimization problem for  $\mathcal{R}_{\alpha, \Gamma}^\kappa$  is reduced to the inequality  $C_L^1(u)$  being thus proved.

*Remark:* The (reverse) inequalities hold also for  $p \in [-2, 0)$  showing, e.g., that a *charged loop in the absence of gravity takes a circular form*.



# A discrete analogue: polymer loops



Consider the same loop as above with *point interactions* placed at the *arc distances*  $\frac{jL}{N}$ ,  $j = 0, \dots, N_1$ , in other words, the formal Hamiltonian

$$H_{\alpha, \Gamma}^N = -\Delta + \tilde{\alpha} \sum_{j=0}^{N-1} \delta\left(x - \Gamma\left(\frac{jL}{N}\right)\right)$$

in  $L^2(\mathbb{R}^d)$ ,  $d = 2, 3$ , where the last term has to be properly defined

We are interested in the shape of  $\Gamma$  which *maximizes* the ground state energy provided, of course, that the discrete spectrum of  $H_{\alpha, \Gamma}^N$  is non-empty; this requirement is *nontrivial for  $d = 3$* .

Introduce the *generalized boundary values* as the coefficients in the expansion of  $H_Y^*$  where  $H_Y$  is the Laplacian restricted to functions vanishing at the vicinity of the points of  $Y$ .

# Point interactions ‘necklaces’



A reminder: fixing the points  $y_j \in Y$  the said expansions look as

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

$$\psi(x) = \frac{1}{4\pi|x - y_j|} L_0(\psi, y_j) + L_1(\psi, y_j) + \mathcal{O}(|x - y_j|), \quad d = 3.$$

*Local* self-adjoint extensions are then given by

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

the absence of interaction corresponds to  $\alpha = \infty$ , for details we refer to



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

## Theorem

The *ground state* of  $H_{\alpha, \Gamma}^N$  is uniquely maximized by a *N-regular polygon*.



P.E.: Necklaces with interacting beads: isoperimetric problems, in Proceedings of the “International Conference on Differential Equations and Mathematical Physics” (Birmingham 2006), AMS *Contemporary Mathematics Series*, vol. 412, Providence, R.I., 2006; pp. 141-149.

# New effects in three dimensions



In three dimensions the discrete spectrum of  $H_{\alpha, \Gamma} = -\Delta - \alpha\delta(x - \Gamma)$  *may be empty* if  $\alpha$  is small enough. Recall the *sphere example* mentioned earlier where bound states are known to exist if and only if  $\alpha R > 1$ .

This raises the following question: given the *critical sphere*,  $\alpha R = 1$ , would its *deformation produce a discrete spectrum*? One answer is

## Theorem

Let  $\Gamma_\epsilon$  be a *deformation of the sphere* expressed in spherical coordinates as  $r(\theta, \phi) = R(1 + \epsilon\rho(\theta, \phi))$  where  $\rho$  is *nonzero function of zero mean*. If  $H_{\alpha, \Gamma_0}$  is *critical*,  $\sigma_{\text{disc}}(H_{\alpha, \Gamma_\epsilon}) \neq \emptyset$  holds for all *nonzero  $\epsilon$  small enough*.



P.E., M. Fraas: On geometric perturbations of critical Schrödinger operators with a surface interaction, *J. Math. Phys.* **50** (2009), 112101.

*Remarks:* (a) The results *fails to hold globally*: if a *surface-preserving* deformation of a critical surface is *elongated enough*, the discrete spectrum is *empty*.

(b) In contrast, deformation of a critical surface *always produces a nonvoid discrete spectrum* if it is *capacity preserving*.

# Cones



We have mentioned *conical surfaces*. To state the question, let  $\mathcal{T}$  be a  $C^2$ -smooth loop on the 2D unit sphere  $\mathbb{S}^2 \subset \mathbb{R}^3$  of length  $|\mathcal{T}|$  without self-intersections. We distinguish between *circular* and *non-circular loops*; a circle  $\mathcal{C} \subset \mathbb{S}^2$  has, of course, the length  $|\mathcal{C}| \leq 2\pi$ .

The  $C^2$ -smooth cone  $\Sigma_R(\mathcal{T}) \subset \mathbb{R}^3$  of radius  $R \in (0, \infty]$  with a  $C^2$ -smooth loop  $\mathcal{T} \subset \mathbb{S}^2$  as its *cross-section* is

$$\Sigma_R(\mathcal{T}) := \{r\mathcal{T} \in \mathbb{R}^3 : r \in [0, R)\};$$

it is called *finite* (or *truncated*) if  $R < \infty$  and *infinite* otherwise.

## Theorem

For finite cones  $\Gamma_R := \Sigma_R(\mathcal{C})$  and  $\Lambda_R := \Sigma_R(\mathcal{T})$  of radius  $R > 0$  with  $L := |\mathcal{C}| = |\mathcal{T}| \in (0, 2\pi]$  we have  $\#\sigma_{\text{disc}}(H_{\alpha, \Gamma_R}) \geq 1$  if and only if  $\alpha > \alpha_{\text{crit}}$  holds for some  $\alpha_{\text{crit}}(L, R) > 0$ . If the loops  $\mathcal{T}$  and  $\mathcal{C}$  are *not congruent*,  $\sigma_{\text{crit}}(H_{\alpha, \Lambda_R})$  is nonempty for  $\alpha \geq \alpha_{\text{crit}}$  and  $\lambda_1(H_{\alpha, \Lambda_R}) < \lambda_1(H_{\alpha, \Gamma_R})$ .



P.E., V. Lotoreichik: A spectral isoperimetric inequality for cones, *Lett. Math. Phys.* **107** (2017), 717–732.

# Cones, continued



In particular, we have the effect we have encountered with spheres:

## Corollary

Any (fixed-radius, smooth, conical) deformation of a *critical* circular cone gives rise to a *non-void discrete spectrum* of the corresponding  $H_{\alpha,\Gamma}$ .

For *infinite cones* the essential spectrum changes,  $\sigma_{\text{ess}}(H_{\alpha,\Gamma}) = [-\frac{1}{4}\alpha^2, \infty)$ , however, the above *spectral inequality* holds again.

These results follow from the generalized BS principle in combination with an inequality related to  $C_L^p(u)$  used earlier: for a  $C^2$ -smooth loop  $\mathcal{T} \subset \mathbb{S}^2$  we put  $\Phi_f[\mathcal{T}] := \int_0^L \int_0^L f(|\tau(s) - \tau(t)|^2) ds dt$ ; then we have

## Proposition

Let  $f \in C([0, \infty); \mathbb{R})$  be *convex and decreasing*. If  $|\mathcal{T}| = |\mathcal{C}| = L$  for some  $L \in (0, 2\pi]$ , then *isoperimetric inequality*  $\Phi_f[\mathcal{C}] < \Phi_f[\mathcal{T}]$  is valid.



G. Lúko: On the mean length of the chords of a closed curve, *Israel J. Math.* 4 (1966), 23–32.



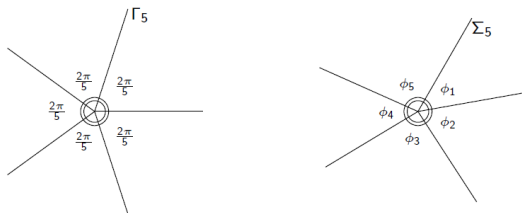
J. O'Hara: *Energy of knots and conformal geometry*, World Scientific 2003.

## Another object of interest: stars



Let us return to planar leaky graphs and consider next *star graphs*  $\Sigma_N = \Sigma_N(L) \subset \mathbb{R}^2$ , which have  $N \geq 2$  edges of length  $L \in (0, \infty]$  each, enumerated in the clockwise manner.

They are characterized by the angles  $\phi = \phi(\Sigma_N) = \{\phi_1, \phi_2, \dots, \phi_N\}$  between the neighboring edges,  $\phi_n \in (0, 2\pi)$  for all  $n \in \{1, \dots, N\}$  and  $\sum_{n=1}^N \phi_n = 2\pi$ ; by  $\Gamma_N$  we denote the star graph with *maximum symmetry*, in other words,  $\phi_n = \frac{2\pi}{N}$  for  $n = 1, \dots, N$ .



The problem can be treated using the same method as before, i.e. a combination of the *generalized BS principle* and *geometric inequalities*.

## Theorem

For  $L < \infty$  and any  $\alpha > 0$  we have the relation

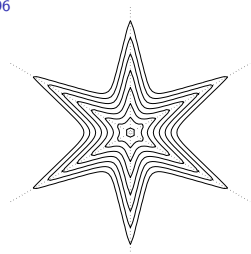
$$\max_{\Sigma_N(L)} \lambda_1^\alpha(\Sigma_N(L)) = \lambda_1^\alpha(\Gamma_N(L)),$$

where the maximum is taken over all star graphs with  $N \geq 2$  edges of; the *equality* is achieved if and only if  $\Sigma_N$  and  $\Gamma_N$  are *congruent*.



P. Exner, V. Lotoreichik: Optimization of the lowest eigenvalue for leaky star graphs, in Proceedings of the conference "Mathematical Results in Quantum Physics" (QMath13, Atlanta 2016; F. Bonetto, D. Borthwick, E. Harrell, M. Loss, eds.), Contemporary Math., vol 717, AMS, Providence, R.I., 2018; pp. 187–196

The analogous result holds for *infinite stars*,  $L = \infty$ . For illustration we show the ground-state eigenfunction for  $\Sigma_6(\infty)$ .



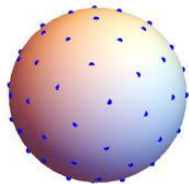
# Stars in three dimensions



Albeit technically nontrivial, the previous problem was simple in the sense that the result was easy to guess.

This would not be the same if we consider an analogue of the star optimization problem *in three dimensions*, i.e. for Schrödinger operators with a singular interaction of  $\text{codim } \Gamma = 2$  supported by a ‘sea urchin’ shape set  $\Gamma$  of  $N$  ‘pins’, finite or semi-infinite.

Optimization problem for 3D stars is no doubt nontrivial. The first analogue coming to mind is the century-old *Thomson problem* about the equilibrium distribution of  $N$  *point charges* on the surface of a sphere.



J.J. Thomson: On the structure of the atom: an investigation of the stability and periods of oscillation of a number of corpuscles arranged at equal intervals around the circumference of a circle; with application of the results to the theory of atomic structure, *Phil. Mag.* **7** (1904), 237–265.



# Inspiration from Thomson problem



Thomson problem is notoriously difficult; recall that a *rigorous* solution is known for a few small  $N$  cases, for instance, a (computer-assisted) proof for  $N = 5$  was presented only recently.



R.E. Schwartz: The five-electron case of Thomson's problem, *Experim. Math.* **22** (2013), 157–186.

Note also that twenty years ago Stephen Smale included it into the list of eighteen '*new Hilbert problems*' for the 21st century.

Attempts to solve it led to generalizations triggering numerous investigations in *algebraic combinatorics*, see for instance



H. Cohen, A. Kumar: Universally optimal distribution of point on the sphere, *J. AMS* **20** (2007), 99–148.



E. Bannai, E. Bannai: A survey on spherical designs and algebraic combinatorics on spheres, *Eur. J. Combin.* **30** (2009), 1392–1425.

Unfortunately – and this makes a theoretical physicist unhappy – *physics is forgotten at that!* They quote, for instance, *Tamme's problem* in botany but not Thomson. The *plum-pudding model* was wrong, of course, but still physics was the original inspiration here!

# Universal optimality by Cohen and Kumar



Consider  $N$  points  $\{x_i\}_{i=1}^N$  living on the unit sphere  $S^2$ . They form an  *$M$ -spherical design* if for any polynomial  $x \mapsto p(x)$  on  $\mathbb{R}^3$  of total degree  $M$  the equivalence one has  $\int_{S^2} p(x) dx = \frac{1}{N} \sum_i^N p(x_i)$  holds.

Let  $m$  be the number of *different inner* products between distinct  $\{x_i\}_{i=1}^N$ . They form a *sharp configuration* if it is  $2m-1$  spherical design.

By [Cohen-Kumar'07, loc.cit.] sharp configurations are *universally optimal* meaning that they minimize *any* potential energy  $f : [0, 4] \rightarrow \mathbb{R}$  which is *completely monotonous*, i.e. it satisfies  $(-1)^k f^{(k)} \geq 0$  for all  $k \geq 0$ . In three dimensions there are *five sharp configurations*:

- $N = 2$ , *antipodal points*
- $N = 3$ , *simplex* with inner product  $-1/2$ ,
- $N = 4$ , *tetrahedron* – simplex with inner product  $-1/3$ ,
- $N = 6$ , *octahedron* – cross polytope with inner products  $-1, 0$ ,
- $N = 12$ , *icosahedron* with inner products  $-1, \pm 1/\sqrt{5}$ .

*Remark:* The remaining Platonic solids, *cube* and *dodekahedron*, do not qualify for universality having  $m=3$  and  $4$ , respectively. Note that they *do not represent Thomson problem solutions either!*

# Application to star leaky graphs



One may wonder what has the mentioned *minimization* problem to do with the *maximization* of the ground state eigenvalues. The answer is that, as in the previously addressed cases, the problem is equivalent to minimization of the (norm of) the *Birman-Schwinger operator*. We have

## Lemma

Consider an *N-arm star* with edges of length  $L \in (0, \infty]$  determined by unit vectors  $\{\bar{\gamma}_i\}_{i=1}^N$ , and let  $\{\bar{\sigma}_i\}_{i=1}^N$  corresponds to a *sharp-configuration star*. Then we have

$$\sum_{i,j \text{ } i \neq j} T_{\kappa;s,t}(|\bar{\gamma}_i - \bar{\gamma}_j|^2) \geq \sum_{i,j \text{ } i \neq j} T_{\kappa;s,t}(|\bar{\sigma}_i - \bar{\sigma}_j|^2).$$

for any  $s, t \in [0, L]$  and the inequality is sharp unless the two stars are *congruent*. Here  $T_{\kappa;s,t}(x) := \frac{e^{-\kappa\sqrt{a+bx}}}{4\pi\sqrt{a+bx}}$  with  $a = (s - t)^2$  and  $b = st$

# Application to star leaky graphs, continued



Next we use the fact that the largest eigenvalue of the Birman-Schwinger operator corresponding to a sharp-configuration star has the *maximum symmetry*,  $\tilde{f}_\sigma = (f_\sigma, \dots, f_\sigma) \in \bigoplus_1^N L^2([0, L])$ .

Then  $\sup Q_{\kappa, \gamma} \geq (Q_{\kappa, \gamma} \tilde{f}_\sigma, \tilde{f}_\sigma) \geq \sup Q_{\kappa, \sigma}$  holds according to the above lemma, which allows us to make the following conclusion:

## Theorem

Assume that  $N \in \{2, 3, 4, 6, 12\}$ , then the ground state energy of the  $N$ -arm leaky star assumes the *unique maximum* for  $\gamma = \sigma$ , where  $\sigma$  is the corresponds to the appropriate sharp configuration listed above.



P.E., S. Kondej: Ground state optimization for leaky star graphs in dimension three, *Lett. Math. Phys.* **110** (2020), 735–751.

For other values of  $N$  the problem remains *open*; note that for a *finite star* the solutions may depend on the coupling constant  $\alpha$ .

# What to bring home from Lecture V



- In the *strong coupling* asymptotic regime leaky quantum structures behave as having effectively a *lower dimension*.
- The *boundaries* of the interaction support have in this regime the *Dirichlet* character.
- *Weakly bound states* due to *geometric perturbations* behave like regular Schrödinger operators, *powerlike* for curves, *exponential* for surfaces.
- If the geometry of the interaction support is *essentially two-dimensional*, the ground state is typically maximized by configurations of *maximum symmetry*.
- If it is *truly three-dimensional*, on the other hand, the optimization problem is considerably more involved.