Constrained quantum dynamics

Pavel Exner

Doppler Institute
for Mathematical Physics and Applied Mathematics
Prague

With thanks to all my collaborators

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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:

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- Another question concerns the asymptotic behavior in the situation when the geometric perturbation of the 'trivial' system is *gentle*.

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- It is even more important to analyze the opposite extremum, the *asymptotic behavior* in the *strong-coupling regime*, $\alpha \to \infty$.
- 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 δ interaction asymptotics

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Theorem

Let Γ be a C^4 smooth curve in $\mathbb{R}^2$ without ends, either a closed loop or infinite, asymtotically straight and without 'near crossings'. In the limit $\alpha \to \infty$ the jth eigenvalue of $H_{\alpha,\Gamma}$ behaves as

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

where μ_j is the jth eigenvalue of $S_\Gamma = -\frac{\mathrm{d}^2}{\mathrm{d}s^2} - \frac{1}{4}\kappa(s)^2$ on $L^2(0, |\Gamma|)$ or $L^2(\mathbb{R})$, respectively, where κ is curvature of Γ.

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

Strong δ interaction asymptotics

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

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

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

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

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

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

- for a *curve in* $\mathbb{R}^2$ we replace $-\frac{1}{4}\alpha^2$ by $\epsilon_\alpha = -4\,\mathrm{e}^{2(-2\pi\alpha+\psi(1))}$.

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

Strong δ interaction asymptotics

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

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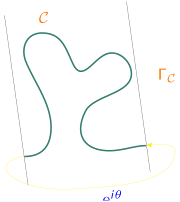
In a similar way one can treat *periodic systems* using the *Blach* (Floquet, Gel'fand) decomposition: there is a unitary $\mathcal{U}$ such that $\mathcal{U} H_{\alpha,\Gamma} \mathcal{U}^{-1} = \int_{[0,2\pi)^r}^{\oplus} H_{\alpha,\theta}\, \mathrm{d}\theta$ and $\sigma(H_{\alpha,\Gamma}) = \bigcup_{[0,2\pi)^r}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



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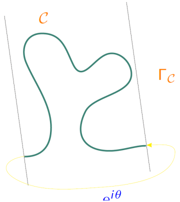
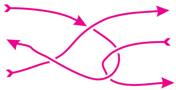


It is important to choose the periodic cells $\mathcal{C}$ of the space and $\Gamma_{\mathcal{C}}$ of the manifold *consistently*, $\Gamma_{\mathcal{C}} = \Gamma \cap \mathcal{C}$. Note that $\Gamma_{\mathcal{C}}$ is not necessarily a 'straight slab', even for $d = 2$, and for $d = 3$ it need not be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



Periodic manifold asymptotics

Theorem

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

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

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

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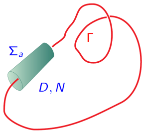
Corollary

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

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

Strong δ interactions: sketch of the argument

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



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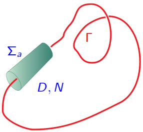

This squeezes $H_{\alpha,\Gamma}$ between a pair of ‘disconnected’ operators, and since we are interested in *negative eigenvalues*, we have to care about the tube part only because the Dirichlet/Neumann Laplacian in the remaining part of $\mathbb{R}^d$ is *positive*.

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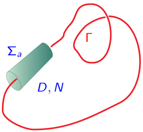

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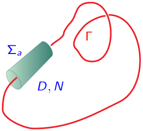

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Then we use inside the tube the *natural curvilinear* (Fermi, parallel) *coordinates* mentioned before, and estimate the coefficients to squeeze $H_{\alpha,\Gamma}$ between operators with *separated variables*. For a curve in $\mathbb{R}^2$, e.g. their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

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

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

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

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

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

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Lemma

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

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

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Finally, we relate a to α by choosing $a = 6\alpha^{-1} \ln \alpha$ which yields the result.

In the other cases the proof is analogous. If $\mathrm{codim}\,\Gamma = 2$ the transverse part is the Dirichlet/Neumann disc of radius r with the point interaction in the center; the error is again exponentially small as $\alpha \to -\infty$.

Curves with ends

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

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Theorem (E-Pankrashkin'14)

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

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

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

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

Curves with ends: sketch of the argument

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

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

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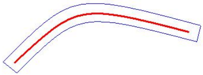
We choose an *'extended' tubular neighborhood*, at each endpoint longer by $a := \frac{6}{\alpha}\ln\alpha$. Now we *loose the advantage of variable separation* but with the help of the above formula one can check that the Neumann condition imposed at this distance from the curve has an effect which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



An extended neighbourhood

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

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

Theorem

Let $H_{\alpha,\Gamma}$ correspond to a finite, non-closed C^4 smooth curve in $\mathbb{R}^3$ with regular ends having length L and the global Frenet frame.

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

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

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

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

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

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

Surfaces with a boundary

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

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We consider again the comparison operator $S_\Gamma = -\Delta_\Gamma^D + K - M^2$, where $-\Delta_\Gamma^D$ is Laplace-Beltrami operator on Γ, now with *Dirichlet condition* at $\partial\Gamma$, and K, M, respectively, are the *Gauss* and *mean* curvatures of Γ

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Theorem

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

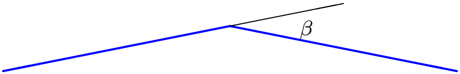
$$\lambda_j(H_{\alpha,\Gamma}) = -\frac{\alpha^2}{4} + \mu_j^D + o(1) \quad \text{as} \quad \alpha \to \infty\,.$$

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

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

Another asymptotics: slightly bent curves

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 β.



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

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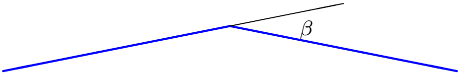

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For slightly bent *Dirichlet tubes* one derives using BS principle that the gap is proportional to the *fourth power* of the bending angle; led by this analogy we conjecture that

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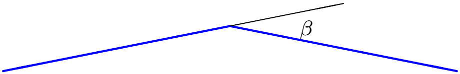

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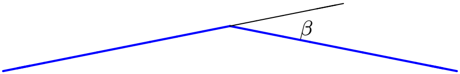

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The question now is (a) what is the coefficient a, and (b) what is the *class of curves* for which such a formula holds.

Weakly bent curves, continued

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

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

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In particular, the *signed curvature* $\gamma(s) = \dot\Gamma_2(s)\ddot\Gamma_1(s) - \dot\Gamma_1(s)\ddot\Gamma_2(s)$ is piecewise continuous and the one-sided limits of $\dot\Gamma$, i.e. *tangent vectors* to the curve at the points of discontinuity exist. We denote them as $\Pi = \{p_i\}_{i=1}^{\sharp\Pi}$ and shall speak of them as of *vertices*. Consequently, Γ consists of $\sharp\Pi + 1$ simple arcs or *edges*, each having as its endpoints one or two of the vertices.

Weakly bent curves, continued

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

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

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

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

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One can reconstruct Γ from $\tilde\gamma$, uniquely up to Euclidean transformations,

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

Weakly bent curves, continued

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

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

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

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

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Lemma

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

Weakly bent curves, the result

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

Theorem

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

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

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

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

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

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

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

Weakly deformed planes

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

The asymptotic expansion

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Theorem

Let $\alpha > 0$ be fixed and set

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

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

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

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

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*.

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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

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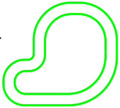
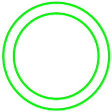
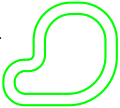
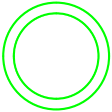
ground state of  $<$ ground state of 

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.

Non-simply connected regions

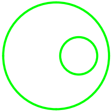
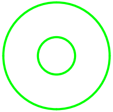
Not always does the intuition tells us the right answer. For instance, the *topology may play role*. Let us mention pictorially two examples in maximum symmetry may lead to *maximum* of the principal eigenvalue If we seek extremum among *strips of fixed length and width* we have

ground state of  $<$ ground state of 

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

ground state of  $<$ ground state of 

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

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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 Γ is congruent with $\mathcal{C}$.

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One more time, we employs 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

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

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 $C_L^p(u)$:

$$\int_0^L |\Gamma(s+u)-\Gamma(s)|^p \mathrm{d}s \le \frac{L^{1+p}}{\pi^p}\, sin^p \frac{\pi u}{L}\,, \quad p>0,\; u\in(0,\tfrac{1}{2}L]$$

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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 $\mathcal{R}^\kappa_{\alpha,\Gamma}$ is reduced to the inequality $C_L^1(u)$ being thus proved.

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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

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

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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

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

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Local self-adjoint extension 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

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Theorem

The ground state of $H^N_{\alpha,\Gamma}$ 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* is α is small enough. Recall the *sphere example* mentioned earlier where bound states are known to exist if and only if $\alpha R > 1$.

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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 $|\mathcal{C}| \le 2\pi$.

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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

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

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

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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 $\#\sigma_{\mathrm{disc}}(H_{\alpha,\Gamma_R}) \geq 1$ if and only if $\alpha > \alpha_{\mathrm{crit}}$ holds for some $\alpha_{\mathrm{crit}}(L, R) > 0$

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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 $H_{\alpha,\Gamma}$.

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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 $\Phi_f[\mathcal{T}] := \int_0^L \int_0^L f(|\tau(s) - \tau(t)|^2)\, \mathrm{d}s\mathrm{d}t$

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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. Lűko: 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.

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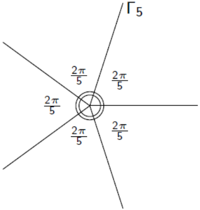

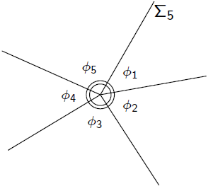

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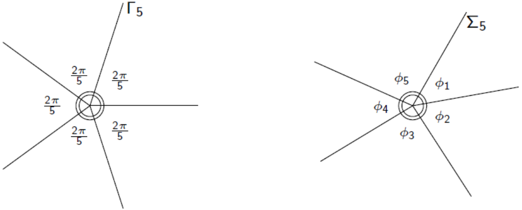

The problem can be treated using the same method as before, i.e. a combination of the *generalized BS principle* and *geometric inequalities*.

Star optimization

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 Σ_N and Γ_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.

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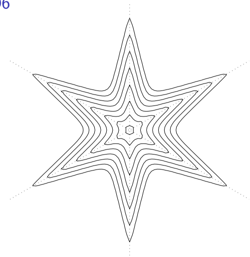
The analogous result holds for *infinite stars*, $L = \infty$. For illustration we show the ground-state eigenfunction for $\Sigma_6(\infty)$.



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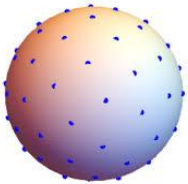
Optimization problem for 3D stars is no doubt nontrivial. The first analogue coming to mind is the century-old *Thomson problem* about the equilibrium distribution of N *point charges* on the surface of a sphere.



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.

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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 $\int_{S^2} p(x)\mathrm{d}x = \frac{1}{N}\sum_i^N p(x_i)$ holds.

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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!*

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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

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

for any $s, t \in [0, L]$ and the inequality is sharp unless the two stars are congruent. Here $T_{\kappa;s,t}(x) := \frac{\mathrm{e}^{-\kappa\sqrt{a+bx}}}{4\pi\sqrt{a+bx}}$ 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*, $\tilde{f}_\sigma = (f_\sigma, \dots, f_\sigma) \in \bigoplus_1^N L^2([0, L])$.

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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:

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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 σ is the corresponds to the appropriate sharp configuration listed above.

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

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- If it is *truly three-dimensional*, on the other hand, the optimization problem is considerably more involved.