Geometric properties of the ground state for Hamiltonians with singular interactions

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Motivation

Relations between *geometry* and *principal eigenvalue* are a traditional question in mathematical physics. Recall, e.g., the *Faber-Krahn inequality* for the Dirichlet Laplacian $-\Delta_D^M$ in a compact $M \subset \mathbb{R}^2$: among all regions with a fixed area the ground state is *uniquely minimized by the circle*,

$$\inf \sigma(-\Delta_D^M) \geq \pi j_{0,1}^2 \, |M|^{-1};$$

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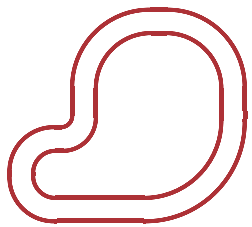
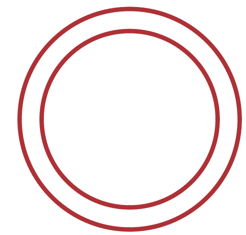
similarly *a ball* is a minimizer for a compact $M \subset \mathbb{R}^d,\ d \geq 3$

Another classical example is the *PPW conjecture* proved by *Ashbaugh* and *Benguria*: in the 2D situation we have

$$\frac{\lambda_2(M)}{\lambda_1(M)} \leq \left(\frac{j_{1,1}}{j_{0,1}}\right)^2$$

Motivation, continued

Symmetry of M may correspond also to the *maximum* of the principal eigenvalue; for instance for *a strip of fixed length and width* [E.-Harrell-Loss'99] we have

ground state of  $<$ ground state of 

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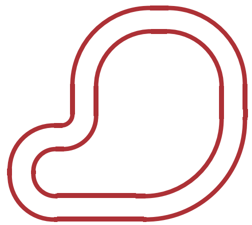
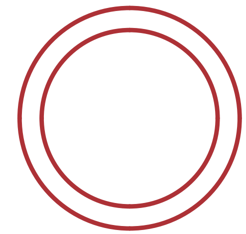
ground state of  $<$ ground state of 

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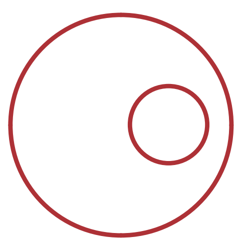
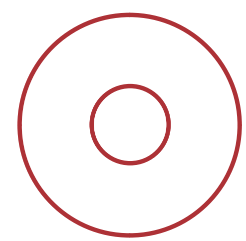
Another example is a *circular obstacle in circular cavity* [Harrell-Kröger-Kurata'01]

ground state of  $<$ ground state of 

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

Motivation, continued

In other cases the geometry concerns rather a *potential configuration*. Recall, for instance, a recent result result of [Baker-Loss-Stolz'08] on the spectral minimum of $-\Delta + V$ in $L^2(\mathbb{R}^d)$ where the potential $V_\omega(x) = \sum_{i\in\mathbb{Z}^d} q(x-i-\omega_i)$

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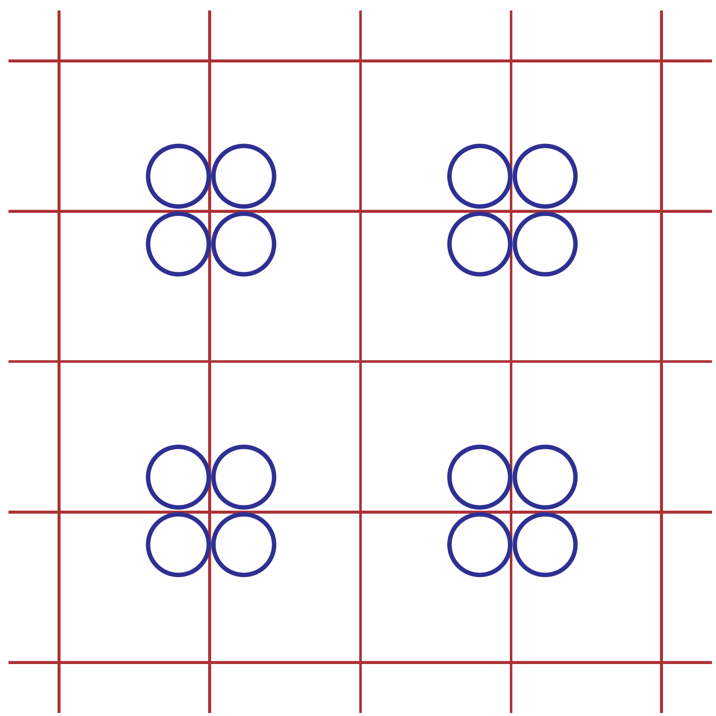
In this case the minimizing configuration is shown to be



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The subject of this talk will be several problems of the above type for *solvable models* of quantum systems, that is, Hamiltonians with *point-* or *contact-type interactions*. Specifically, we will consider

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- *Quantum graphs* with attractive δ coupling at the vertices – dependence on edge lengths
- Finally, *point interactions* in $\mathbb{R}^2$ and $\mathbb{R}^3$ again and their continuous analogue

Polymer loops

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Polymer loops

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The question is the following: we take a closed loop Γ – parametrized in the standard way by its *arc length* – and consider a class of singular Schrödinger operators in $L^2(\mathbb{R}^d),\ d = 2, 3,$ given formally by the expression

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

We are interested in the shape of Γ which *maximizes* the ground state energy provided, of course, that the discrete spectrum of $H^N_{\alpha,\Gamma}$ is non-empty.

A reminder: 2D point interactions

Fixing the site y_j and “coupling constant” α we define them by b.c. which change *locally* the domain of $-\Delta$: we require

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

where the generalized b.v. $L_0(\psi, y_j)$ and $L_1(\psi, y_j)$ satisfy

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

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For $Y_\Gamma := \{y_j := \Gamma\left(\frac{jL}{N}\right) :\, j=0,\dots,N-1\}$ we define in this way $-\Delta_{\alpha,Y_\Gamma}$ in $L^2(\mathbb{R}^2)$. It holds $\sigma_{\mathrm{disc}}\left(-\Delta_{\alpha,Y_\Gamma}\right) \neq \emptyset$, i.e.

$$\epsilon_1 \equiv \epsilon_1(\alpha,Y_\Gamma) := \inf\sigma\left(-\Delta_{\alpha,Y_\Gamma}\right) < 0\,,$$

which is always true in two dimensions – cf. [AGHH'88, 05]

A reminder: 3D point interactions

Similarly, for y_j and “coupling” α we define them by b.c. which change locally the domain of $-\Delta$: we require

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

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

giving $-\Delta_{\alpha,Y_\Gamma}$ in $L^2(\mathbb{R}^3)$. However, $\sigma_{\mathrm{disc}}\left(-\Delta_{\alpha,Y_\Gamma}\right) \neq \emptyset$, i.e.

$$\epsilon_1 \equiv \epsilon_1(\alpha, Y_\Gamma) := \inf \sigma\left(-\Delta_{\alpha,Y_\Gamma}\right) < 0\,,$$

is now a nontrivial requirement; it holds only for α below some critical value α_0 – cf. [AGHH'88, 05]

A geometric reformulation

By Krein's formula, the spectral condition is reduced to an algebraic problem. Using $k = i\kappa$ with $\kappa > 0$, we find the ev's $-\kappa^2$ of our operator from

$$\det \Gamma_k = 0 \quad \text{with} \quad (\Gamma_k)_{ij} := (\alpha - \xi^k)\delta_{ij} - (1-\delta_{ij})g_{ij}^k \,,$$

where the off-diagonal elements are $g_{ij}^k := G_k(y_i - y_j)$, or equivalently

$$g_{ij}^k = \frac{1}{2\pi} K_0(\kappa|y_i - y_j|)$$

and the regularized Green's function at the interaction site is

$$\xi^k = -\frac{1}{2\pi}\left(\ln\frac{\kappa}{2} + \gamma_{\mathrm{E}}\right)$$

Geometric reformulation, continued

The ground state refers to the point where the *lowest* ev of $\Gamma_{i\kappa}$ vanishes. Using smoothness and monotonicity of the κ-dependence we have to check that

$$\min \sigma(\Gamma_{i\tilde{\kappa}_1}) < \min \sigma(\tilde{\Gamma}_{i\tilde{\kappa}_1})$$

holds locally for $\Gamma \neq \tilde{\mathcal{P}}_N$, where $-\tilde{\kappa}_1^2 := \epsilon_1(\alpha, \tilde{\mathcal{P}}_N)$

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There is a *one-to-one relation* between an ef $c = (c_1, \dots, c_N)$ of $\Gamma_{i\kappa}$ at that point and the corresponding ef of $-\Delta_{\alpha,\Gamma}$ given by $c \leftrightarrow \sum_{j=1}^N c_j G_{i\kappa}(\cdot - y_j)$, up to normalization. In particular, the lowest ev of $\tilde\Gamma_{i\tilde\kappa_1}$ corresponds to the eigenvector $\tilde\phi_1 = N^{-1/2}(1, \dots, 1)$; hence the spectral threshold is

$$\min \sigma(\tilde\Gamma_{i\tilde\kappa_1}) = (\tilde\phi_1, \tilde\Gamma_{i\tilde\kappa_1}\tilde\phi_1) = \alpha - \xi^{i\tilde\kappa_1} - \frac{2}{N}\sum_{i<j} \tilde g_{ij}^{i\tilde\kappa_1}$$

Geometric reformulation, continued

On the other hand, we have $\min \sigma(\Gamma_{i\tilde{\kappa}_1}) \leq (\tilde{\phi}_1, \Gamma_{i\tilde{\kappa}_1}\tilde{\phi}_1)$, and therefore it is sufficient to check that

$$\sum_{i<j} G_{i\kappa}(y_i - y_j) > \sum_{i<j} G_{i\kappa}(\tilde{y}_i - \tilde{y}_j)$$

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holds *for all* $\kappa > 0$ and $\Gamma \neq \tilde{\mathcal{P}}_N$. Call $\ell_{ij} := |y_i - y_j|$ and $\tilde{\ell}_{ij} := |\tilde{y}_i - \tilde{y}_j|$ and define $F : \ (\mathbb{R}_+)^{N(N-3)/2} \to \mathbb{R}$ by

$$F(\{\ell_{ij}\}) := \sum_{m=2}^{[N/2]} \sum_{|i-j|=m} \left[G_{i\kappa}(\ell_{ij}) - G_{i\kappa}(\tilde{\ell}_{ij}) \right] ;$$

Using the *convexity* of $G_{i\kappa}(\cdot)$ for a fixed $\kappa > 0$ we get

$$F(\{\ell_{ij}\}) \geq \sum_{m=2}^{[N/2]} \nu_m \left[G_{i\kappa}\left(\frac{1}{\nu_m} \sum_{|i-j|=m} \ell_{ij} \right) - G_{i\kappa}(\tilde{\ell}_{1,1+m}) \right] ,$$

where ν_n is the number of the appropriate chords

Geometric reformulation, continued

It is easy to see that

$$\nu_m := \begin{cases} N & \dots \qquad m = 1, \dots, \left[\frac{1}{2}(N-1)\right] \\ \frac{1}{2}N & \dots \qquad m = \frac{1}{2}N \quad \text{for } N \text{ even} \end{cases}$$

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Since $G_{i\kappa}(\cdot)$ is also *monotonously decreasing* in $(0, \infty)$, we thus need only to demonstrate that

$$\tilde{\ell}_{1,m+1} \geq \frac{1}{\nu_n} \sum_{|i-j|=m} \ell_{ij}$$

with the sharp inequality for at least one m if $\mathcal{P}_N \neq \tilde{\mathcal{P}}_N$.
In this way the problem becomes again purely geometric

Chord inequalities

Recall that for $\Gamma:\ [0,L]\to\mathbb{R}^d$ we have used the notation

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$$y_j := \Gamma\left(\frac{jL}{N}\right), \quad j = 0, 1, \dots, N-1\,;$$

For fixed $L > 0$, N and $m = 1, \dots, [\frac{1}{2}N]$ we consider the following inequalities for ℓ^p norms related to the chord lengths, that is, the quantities $\Gamma\left(\cdot + \frac{jL}{N}\right) - \Gamma(\cdot)$

$$D^p_{L,N}(m): \quad \sum_{n=1}^N |y_{n+m} - y_n|^p \le \frac{N^{1-p} L^p \sin^p \frac{\pi m}{N}}{\sin^p \frac{\pi}{N}}\,, \quad p > 0\,,$$

$$D^{-p}_{L,N}(m): \quad \sum_{n=1}^N |y_{n+m} - y_n|^{-p} \ge \frac{N^{1+p} \sin^p \frac{\pi}{N}}{L^p \sin^p \frac{\pi m}{N}}\,, \quad p > 0\,.$$

The *rhs*'s correspond to regular planar polygon $\tilde{\mathcal{P}}_N$

More on the inequalities

In general, the inequalities *are not valid for $p > 2$* as the example of a rhomboid shows: $D^p_{L,4}(2)$ is equivalent to $\sin^p \phi + \cos^p \phi \le 2^{1-(p/2)}$ for $0 < \phi < \pi$ which obviously holds for $p \le 2$ only

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Proposition: $D^p_{L,N}(m) \Rightarrow D^{p'}_{L,N}(m)$ if $p > p' > 0$ and $D^p_{L,N}(m) \Rightarrow D^{-p}_{L,N}(m)$ for any $p > 0$

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Theorem [E'05b]: The inequality $D^2_{L,N}(m)$ is valid

Remark: The inequalities have "continuous" analogues [E-Harrell-Loss'05] with the summation replaced by integration; the *rhs*'s are in this case $L^{1\pm p}\pi^{\mp p} \sin^p \frac{\pi u}{L}$ referring to a circle

Proof of $D^2_{L,N}(m)$

It is clear that one has to deal with case $p = 2$ only. We put $L = 2\pi$ and express Γ through its Fourier series,

$$\Gamma(s) = \sum_{0 \neq n \in \mathbb{Z}} c_n \,\mathrm{e}^{ins}$$

with $c_n \in \mathbb{C}^d$; since $\Gamma(s) \in \mathbb{R}^d$ one has to require $c_{-n} = \bar{c}_n$. We are free to choose $c_0 = 0$ and the normalization condition $\sum_{0 \neq n \in \mathbb{Z}} n^2 |c_n|^2 = 1$ follows from $|\dot{\Gamma}(s)| = 1$

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On the other hand, the left-hand side of $D^2_{2\pi,N}(m)$ equals

$$\sum_{n=1}^{N} \sum_{0\neq j,k\in\mathbb{Z}} c_j^*\cdot c_k \left(\mathrm{e}^{-2\pi imj/N}-1\right)\left(\mathrm{e}^{2\pi imk/N}-1\right)\mathrm{e}^{2\pi in(k-j)/N}$$

Proof of $D^2_{L,N}(m)$, continued

Next we change the order of summation and observe that $\sum_{n=1}^{N} \mathrm{e}^{2\pi i n(k-j)/N} = N$ if $j = k \pmod N$ and zero otherwise; this allows us to write the last expression as

$$4N \sum_{l\in\mathbb{Z}} \sum_{\substack{0 \neq j,k \in \mathbb{Z} \\ j-k=lN}} |j|c_j^* \cdot |k|c_k \left| j^{-1} \sin\frac{\pi m j}{N} \right| \left| k^{-1} \sin\frac{\pi m k}{N} \right| .$$

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Hence the sought inequality $D^2_{2\pi,N}(m)$ is equivalent to

$$\left(d, (A^{(N,m)}\otimes I)d\right) \leq \left(\frac{\pi\sin\frac{\pi m}{N}}{N\sin\frac{\pi}{N}}\right)^2$$

Proof of $D^2_{L,N}(m)$, continued

Here the vector $d \in \ell^2(\mathbb{Z}) \otimes \mathbb{C}^d$ has the components $d_j := |j| c_j$ and the operator $A^{(N,m)}$ on $\ell^2(\mathbb{Z})$ is defined as

$$A^{(N,m)}_{jk} := \begin{cases} \left|j^{-1} \sin \frac{\pi m j}{N}\right| \, \left|k^{-1} \sin \frac{\pi m k}{N}\right| & \text{if} \quad 0 \neq j, k \in \mathbb{Z},\ j - k = lN \\ 0 & \text{otherwise} \end{cases}$$

$A^{(N,m)}$ is obviously bounded because its Hilbert-Schmidt norm is finite; we have to estimate its norm

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Remark: The "continuous" analogue corresponds formally to $N = \infty$. Then $A^{(N,m)}$ is *a multiple of* I and it is only necessary to employ $|\sin jx| \le j \, \sin x$ for any $j \in \mathbb{N}$ and $x \in (0, \frac{1}{2}\pi]$. Here due to *infinitely many side diagonals* such a simple estimate yields an unbounded Toeplitz-type operator, and one has use the *matrix-element decay*

Proof of $D^2_{L,N}(m)$, continued

For a given $j \neq 0$ and $d \in \ell^2(\mathbb{Z})$ we have

$$\left(A^{(N,m)} d\right)_j = \left| j^{-1} \sin \frac{\pi m j}{N} \right| \sum_{\substack{0 \neq k \in \mathbb{Z} \\ k = j (\operatorname{mod} N)}} \left| k^{-1} \sin \frac{\pi m k}{N} \right| d_k$$

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The norm $\|A^{(N,m)}d\|$ is then easily estimated by means of Schwarz inequality,

$$\begin{aligned} \|A^{(N,m)}d\|^2 &= \sum_{0\neq j\in\mathbb{Z}} j^{-2}\sin^2\frac{\pi m j}{N} \left| \sum_{\substack{0 \neq k \in \mathbb{Z} \\ k = j (\mathrm{mod}\, N)}} \left|k^{-1}\sin\frac{\pi m k}{N}\right| d_k \right|^2 \\ &\leq \sum_{n=0}^{N-1} \sin^4\frac{\pi m n}{N}\, S_n^2 \sum_{\substack{n+lN \neq 0 \\ l \in \mathbb{Z}}} |d_{n+lN}|^2 \end{aligned}$$

Proof of $D^2_{L,N}(m)$, concluded

Here we have introduced

$$S_n := \sum_{\substack{n+lN\neq 0\\ l\in\mathbb{Z}}} \frac{1}{(n+lN)^2} = \sum_{l=1}^{\infty}\left\{\frac{1}{(lN-n)^2}+\frac{1}{(lN-N+n)^2}\right\}$$

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The sought claim, the validity of $D^2_{L,N}(m)$, then follows from

$$\sin\frac{\pi m}{N}\sin\frac{\pi r}{N} > \left|\sin\frac{\pi}{N}\sin\frac{\pi m r}{N}\right|, \quad 2\le r<m\le\left[\frac{1}{2}N\right]$$

This can be also equivalently written as the inequalities $U_{m-1}\left(\cos\frac{\pi}{N}\right) > \left|U_{m-1}\left(\cos\frac{\pi r}{N}\right)\right|$ for Chebyshev polynomials of the second kind; they are verified directly $\square$

Remarks

- Also the spectral result has *continuous analogue*: consider the singular Schrödinger operator

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

in $L^2(\mathbb{R}^2)$, where Γ is a loop of fixed length in the plane; we suppose that it has no *zero-angle* self-intersections. The *principal eigenvalue is maximized if Γ is a circle.* The proof is similar as above but somewhat simpler

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- The inequalities have also other applications. Consider N equal point charges attached at equal distances to a loop. By $D_{L,N}^{-1}(m)$ such an electrostatic problem has planar polygon $\tilde{\mathcal{P}}_N$ as its *unique minimizer*

Point interaction in a bounded region

Our next question concerns the operator written formally as

$$-\Delta_D^\Omega + \tilde{\alpha}\delta(x - x_0)$$

where $\Omega \subset \mathbb{R}^d$ is a precompact set; we ask about optimization of the principal eigenvalue w.r.t. the point-interaction site x_0

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For the moment we consider $d = 2, 3$ leaving out the one-dimensional situation which has its specifics

- variation of Ω has a different character
- the answer may depend on the coupling sign

More about that a little later

Green's function

We assume that Ω is bounded and connected with piecewise C^1 boundary, then $-\Delta_D^\Omega$ has a purely discrete spectrum which allows us to write the Green function

$$\mathcal{G}_0^z(\vec{x},\vec{x}\,') = \sum_{n\in\mathbb{N}_0,\,k\le N_n} \frac{\psi_{n,k}(\vec{x}\,')\,\psi_{n,k}(\vec{x})}{\lambda_n+z}$$

where N_n is the multiplicity of the n-th eigenvalue

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where N_n is the multiplicity of the n-th eigenvalue

Note that it has the same diagonal singularity as the corresponding Green's function in the whole $\mathbb{R}^d$,

$$\mathcal{G}^z(\vec{x},\vec{x}') = \frac{1}{2\pi} K_0(\sqrt{z}\,|\vec{x}-\vec{x}'|) \quad \text{and} \quad e^{-\sqrt{z}|\vec{x}-\vec{x}'|} 4\pi\,|\vec{x}-\vec{x}'|$$

for $d = 2, 3$, respectively. This motivates us to define $h(\cdot,\cdot,\sqrt{z})$ by $\mathcal{G}_0^z(\vec{x},\vec{x}') = \mathcal{G}^z(\vec{x},\vec{x}') - h(\vec{x},\vec{x}',\sqrt{z})$

Spectral condition

The function h is regular and solves the b.v. problem

$$\left\{ \begin{array}{l} (-\Delta + z)\, h(\vec{x}, \vec{x}', \sqrt{z}) = 0 \\ h(\vec{x}, \vec{x}', \sqrt{z})|_{\vec{x}\in\partial\Omega} = \mathcal{G}^z(\vec{x}, \vec{x}')|_{\vec{x}\in\partial\Omega} \end{array} \right. \quad \text{for any} \;\; \vec{x}' \in \Omega$$

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Using it we can find principal ev ξ from the condition

$$\alpha - \ln\sqrt{-\xi} - 2\pi\, h(\vec{x}_0, \vec{x}_0, \sqrt{-\xi}) = 0\,, \qquad \Omega \subset \mathbb{R}^2$$

$$\alpha + \frac{\sqrt{-\xi}}{4\pi} + h(\vec{x}_0, \vec{x}_0, \sqrt{-\xi}) = 0\,, \qquad \Omega \subset \mathbb{R}^3$$

Remarks

The above spectral condition determines all ev's except of those for which $\psi_{\bar{n}}(\vec{x}_0) = 0$ which, however, cannot happen in the ground state

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Lemma: Let λ_0 be the first ev of $-\Delta_\Omega^D$ corresponding to a domain $\Omega \subset \mathbb{R}^3$. For any $\alpha \in \mathbb{R}$, the equation

$$\alpha + \frac{\sqrt{-\xi}}{4\pi} + h(\vec{x}_0, \vec{x}_0, \sqrt{-\xi}) = 0\,, \quad \xi \in (-\infty, \lambda_0)$$

admits a unique solution $\xi(\alpha)$ such that

$$\lim_{\alpha\to-\infty} \xi(\alpha) = -\infty\,, \quad \xi(-h(\vec{x}_0, \vec{x}_0, 0)) = 0\,, \quad \lim_{\alpha\to+\infty} \xi(\alpha) = \lambda_0$$

The same is true for $\Omega \subset \mathbb{R}^2$ except for the middle condition replaced now by $\xi(f(\vec{x}_0, \vec{x}_0, 0)) = 0$ where

$$f(\vec{x}, \vec{x}_0, \sqrt{-\xi}) = 2\pi\, h(\vec{x}, \vec{x}_0, \sqrt{-\xi}) + \ln\sqrt{-\xi}\, I_0(\sqrt{-\xi}\; |\vec{x} - \vec{x}_0|)\,, \quad \xi < \lambda_0$$

Interior reflection property

Definition: Consider a hyperplane P of dimension $d-1$ in $\mathbb{R}^d$ and denote by S^P the mirror image of a set $S \subset \mathbb{R}^d$ w.r.t. P provided $S \cap P = \emptyset$. The domain Ω is said to have the *interior reflection* property w.r.t. P if $P \cap \Omega \neq \emptyset$ and there is an open connected component $\Omega_s \subset \Omega \backslash P$ such that Ω_s^P is a proper subset of $\Omega \backslash \bar{\Omega}_s$. We call Ω_s the *smaller side* of Ω and P an *interior reflection* hyperplane.

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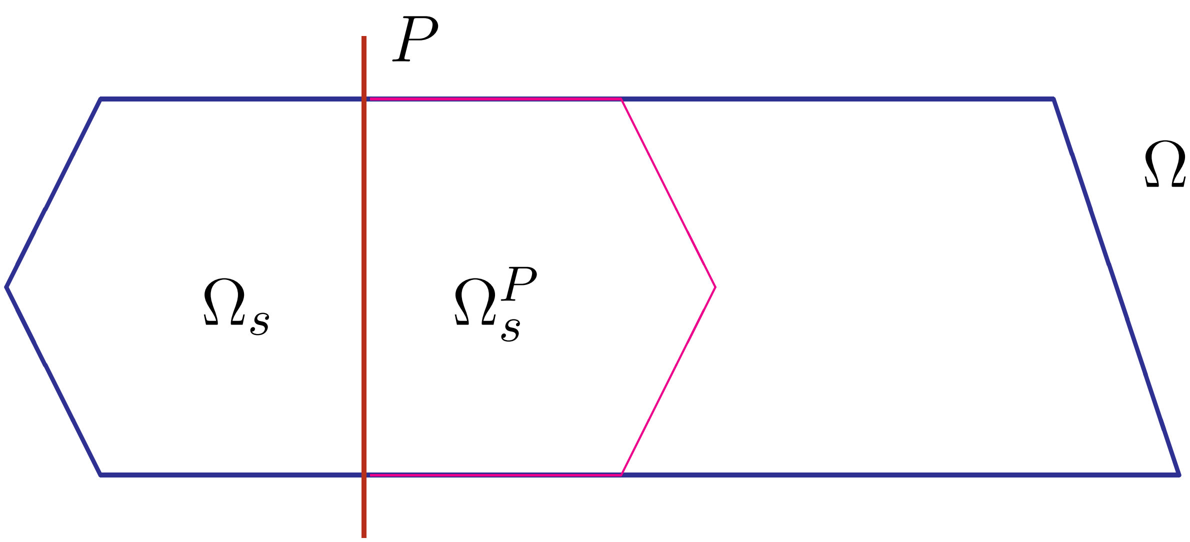

Principal eigenvalue monotonicity

Theorem [E-Mantile'08]: Let P be an interior reflection hyperplane for Ω and $\vec{n}$ the normal vector to P pointing towards Ω_s. Assume that $\vec{x}_0 \in \Omega \cap (\partial\Omega_s \cap P)$; then the principal eigenvalue ξ of H_α with perturbation placed at $\vec{x}_0$ satisfies

$$\vec{n} \cdot \nabla_{\vec{x}_0} \xi > 0$$

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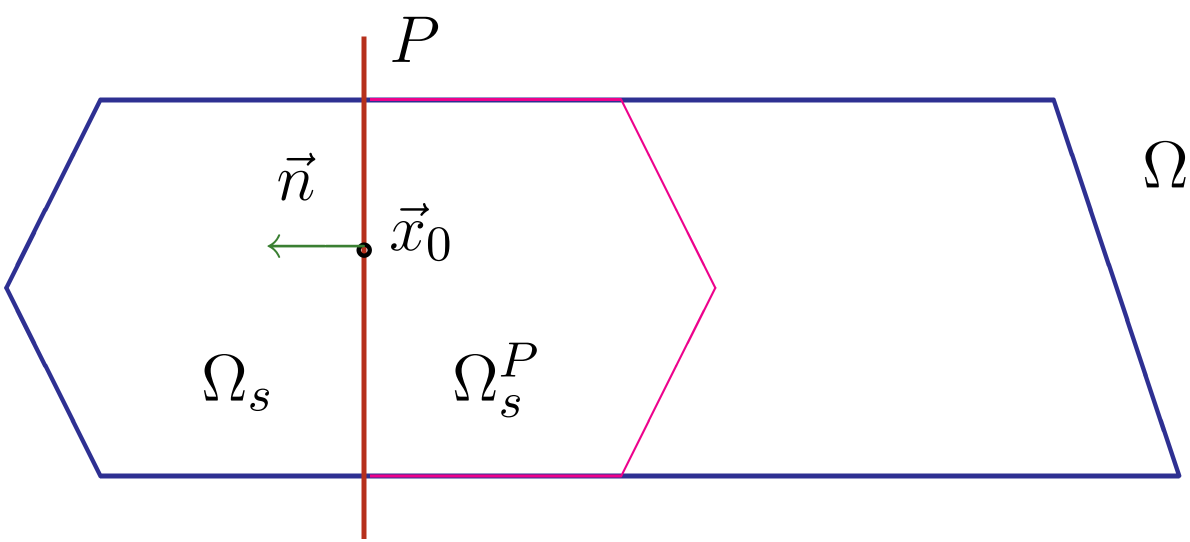

Proof idea

The spectral condition is an implicit equation for ξ; the derivative sign is related to gradient of the function $h(\cdot,\cdot,y)$. The problem can be reduced to analysis of the function u defined on Ω_s by

$$u(\vec{x},\vec{x}_0,y) := h(\vec{x},\vec{x}_0,y) - h(\vec{x}^P,\vec{x}_0,y), \quad \vec{x}\in\Omega_s\,,$$

where $\vec{x}^P$ denotes the mirror image of $\vec{x}\in\Omega_s$ through the plane P. The function u solves the problem

$$\left\{ \begin{array}{l} \left(-\Delta+y^2\right)u = 0 \qquad \text{in } \Omega_s \\ u|_{P\cap\Omega} = 0\,, \quad u|_{\partial\Omega_s\cap\partial\Omega} = \frac{e^{-y|\vec{x}-\vec{x}_0|}}{4\pi|\vec{x}-\vec{x}_0|} - h(\vec{x}^P,\vec{x}_0,y)\Big|_{\vec{x}\in\partial\Omega s\cap\partial\Omega} \end{array} \right. ;\ \vec{x}_0\in\Omega\cap P$$

which allows us to apply Hopf boundary point lemma (about superharmonic functions vanishing at a boundary point) and to translate the conclusion back to h and ξ

Optimization of $\xi(\vec{x}_0)$

For simplicity, consider a convex Ω. Let Π be the set of all the hyperplanes P of interior reflection for Ω; we denote by $\Omega_{s,P}$ the smaller part related to $P \in \Pi$, provided it exists, and set

$$\Sigma := \bigcup_{P \in \Pi} \Omega_{s,P}$$

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Corollary: Let $\Omega \subset \mathbb{R}^d,\ d = 2, 3,$ be an open convex domain, and H_α as defined above with the perturbation at $\vec{x}_0$. The principal eigenvalue of H_α takes its minimum value when $\vec{x}_0$ belongs to the set $\Omega \setminus \Sigma$.

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Examples: disc, elliptic disc, ball, ellipsoid — the minimum is reached with the point interaction at the centre; with less symmetry $\Omega \setminus \Sigma$ may be of nonzero dimension $d_\Omega \leq d$

Remarks

- A similar result can be proved also for *non-convex* domains where interior reflection may give rise to more than one smaller part

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- Note that the result is *independent* of the point interaction coupling parameter α
- One can compare with [Harrell-Kröger-Kurata'01 who proved that for a hard-wall obstacle the principal eigenvalue *decreases* as it moves towards the boundary. The difference is in the different boundary conditions: the hard obstacle is characterized by Dirichlet b.c., while H_α can be obtained as the norm-resolvent limit of a family of sphere interactions Hamiltonians $H_\alpha(r)$ with the b.c. of a *mixed type* as the radius $r \to 0$

ompare: 1D δ interaction in a potential we

Things may look differently if a Dirichlet billiard is replaced by a potential well. Consider a one-dimensional situation

$$H_{\alpha,V,y} = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x) + \alpha\delta(x-y)$$

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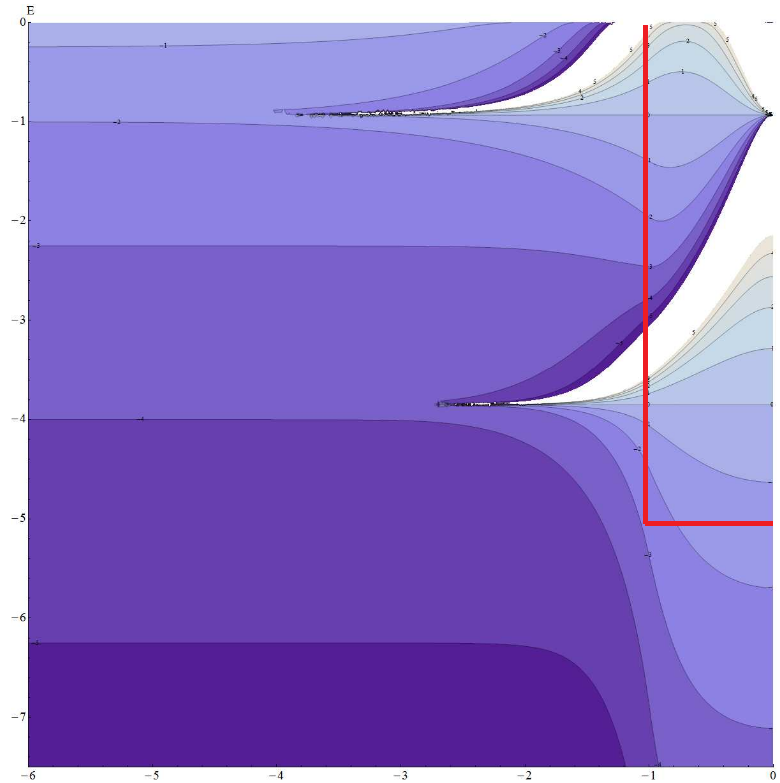
First, $\operatorname{sgn}\alpha$ *matters here* as example of rectangular V shows



Symmetry matters

Consider thus attractive interactions only supposing $\alpha < 0$

In general the optimal δ placement may not coincide with the potential minimum. As example, take the potential

$$V(x) = -c_- x\, \chi_{(-\infty,0]}(x) + c_+ x\, \chi_{[0,-\infty)}(x)$$

with $c_+ \neq c_-$ in general

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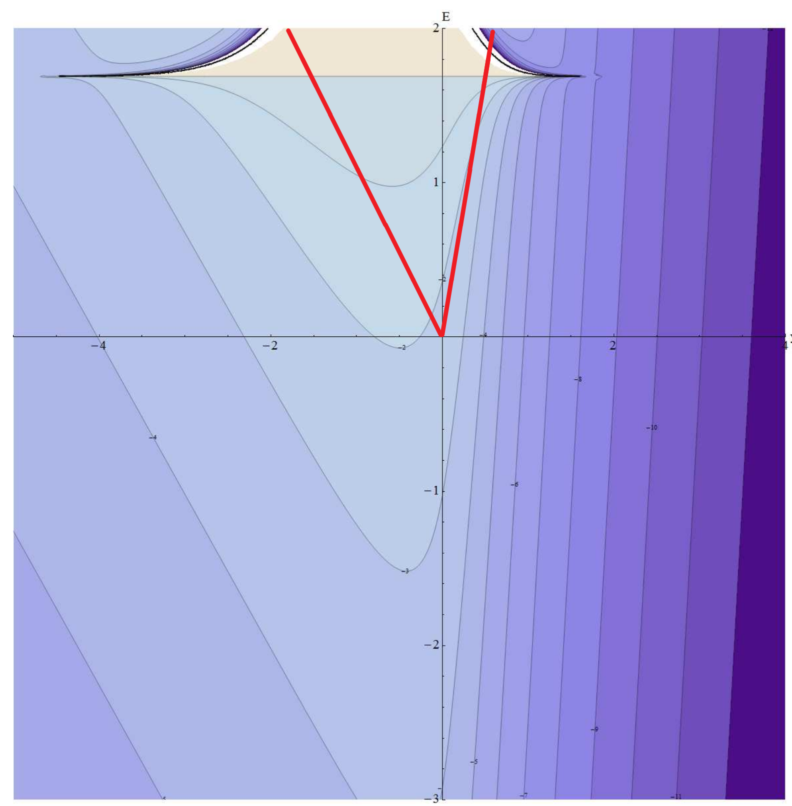

A symmetric potential well

Proposition: Let $V \in C^1$ be even and monotonous in $(0, \infty)$ with $V(0) = 0$. If the principal eigenvalues of both operators are negative we have

$$\inf \sigma(H_{\alpha,V,y_1}) < \inf \sigma(H_{\alpha,V,y_2}) \quad \text{if} \quad |y_1| < |y_2|$$

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Sketch of the proof: Without loss we assume $y_2 > y_1 \geq 0$. Let $\lambda(y)$ and ϕ_y be the ground state *ev* and *ef*, respectively

Using convexity/concavity we check that $\phi_y(x) > \phi_y(-x)$ holds for $x > 0$, so the claim follows by Hellmann-Feynman

$$\frac{\mathrm{d}\lambda(y)}{\mathrm{d}y} = \int_{\mathbb{R}} \frac{\mathrm{d}V(y)}{\mathrm{d}y}\Big|_{y=x} |\phi_y(x)|^2 \mathrm{d}x = \int_0^\infty \frac{\mathrm{d}V(x)}{\mathrm{d}x} \big(|\phi_y(x)|^2 - |\phi_y(-x)|^2\big) \mathrm{d}x > 0$$

One dimension: attractive δ's on the line

Consider Hamiltonian of the form $-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \sum_{j=1}^{n} \alpha_j \delta(x - y_j)$. Defined rigorously [AGHH'08] it is denoted as $-\Delta_{\alpha,Y}$ where $\alpha := \{\alpha_1, \dots, \alpha_n\}$ and $Y := \{y_1, \dots, y_n\}$.

We suppose that all y_j's are mutually distinct and the interactions are attractive, $\alpha_j < 0$, $j = 1, \dots, n$. Then $\sigma_{\mathrm{cont}}(-\Delta_{\alpha,Y}) = \mathbb{R}_+$ and $\sigma_{\mathrm{disc}}(-\Delta_{\alpha,Y}) \subset \mathbb{R}_-$ is non-empty. In particular, there is a ground-state eigenvalue $\lambda_0 < 0$ with a strictly positive eigenfunction ψ_0; we ask how does λ_0 depend on the geometry of the set Y.

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Proposition: Let $\sharp Y_1 = \sharp Y_2$ and $y_{j,1} < y_{j,2} < \dots < y_{j,n}$. Suppose there is an i such that $y_{2,j} = y_{1,j}$ for $j = 1, \dots, i$ and $y_{2,j} = y_{1,j} + \eta$ for $j = i+1, \dots, n$. Assume further that $\psi_0'(y_i+) < 0$ and $\psi_0'(y_{i+1}-) > 0$. Then we have $\min \sigma(-\Delta_{\alpha,Y_1}) \le \min \sigma(-\Delta_{\alpha,Y_2})$ for any $\eta > 0$.

Proof by bracketing

Since $\psi_0 > 0$ and $\psi'' = -\lambda_0\psi$ between the points y_j, the function is convex; by assumption there is $x_0 \in (y_i, y_{i+1})$ such that $\psi_0'(x_0) = 0$. Consider the operator $-\tilde{\Delta}_{\alpha,Y_1}$ which acts as $-\Delta_{\alpha,Y_1}$ with the additional Neumann condition at x_0

We have $-\tilde{\Delta}_{\alpha,Y_1} = -\tilde{\Delta}^l_{\alpha,Y_1} \oplus -\tilde{\Delta}^r_{\alpha,Y_1}$ and the two operators have obviously the same ground state. Consider now the operator $-\hat{\Delta}_{\alpha,Y_2} := -\tilde{\Delta}^l_{\alpha,Y_1} \oplus -\Delta_N \oplus -\tilde{\Delta}^r_{\alpha,Y_1}$ where the added operator is the Neumann Laplacian on $L^2(0,\eta)$; it is clear that the latter does not contribute to the negative spectrum, hence $\min\sigma(-\hat{\Delta}_{\alpha,Y_2}) = \min\sigma(-\tilde{\Delta}_{\alpha,Y_1})$

Furthermore, $-\hat{\Delta}_{\alpha,Y_2}$ is obviously unitarily equivalent to $-\tilde{\Delta}_{\alpha,Y_2}$ with added Neumann conditions at $x = x_0, x_0+\eta$, hence the result follows by Neumann bracketing $\square$

A stronger result

It is easy to see that the derivative-sign assumption is satisfied if $-\alpha_i, -\alpha_{i+1}$ are large enough or, which is the same by scaling, the distance $y_{i+1} - y_i$ is large enough. However, we can make a stronger claim

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Theorem [E-Jex'12]: Suppose again $\sharp Y_1 = \sharp Y_2$ and $\alpha_j < 0$ for all j. Let further $y_{1,i} - y_{1,j} \le y_{2,i} - y_{2,j}$ hold for all i, j and $y_{1,i} - y_{1,j} < y_{2,i} - y_{2,j}$ for at least one pair of i, j, then we have $\min \sigma(-\Delta_{\alpha,Y_1}) < \min \sigma(-\Delta_{\alpha,Y_2})$

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Proof: We employ Krein's formula which makes it possible to reduce the spectral problem at energy k^2 to solution of the secular equation, $\det\Gamma_{\alpha,Y}(\kappa) = 0$, where

$$[\Gamma_{\alpha,Y}(k)]_{jj'} = -[\alpha_j^{-1}\delta_{jj'} + G_k(y_j - y_{j'})]_{j,j'=1}^N$$

and $G_k(y_j - y_{j'}) = \frac{i}{2k}\mathrm{e}^{ik\left|y_j - y_{j'}\right|}$ is the free resolvent kernel

Proof by Krein's formula

Writing $k = i\kappa$ with $\kappa > 0$, we have to investigate the *lowest* eigenvalue of $\Gamma_{\alpha,Y}(\kappa)$ which is, of course, given by

$$\mu_0(\alpha, Y; \kappa) = \min_{|c|=1} \big(c, \Gamma_{\alpha,Y}(\kappa)c\big)\,;$$

the ground state energy $-\kappa^2$ corresponds to κ such that $\mu_0(\alpha, Y; \kappa) = 0$. We set $\ell_{ij} := |y_i - y_j|$, then the quantity to be minimized is explicitly

$$\big(c, \Gamma_{\alpha,Y}(\kappa)c\big) = \sum_{i=1}^{n} |c_i|^2 \left(-\frac{1}{\alpha_i} - \frac{1}{2\kappa}\right) - 2\sum_{i=1}^{n}\sum_{j=1}^{i-1} \mathrm{Re}\,\bar{c}_i c_j \frac{\mathrm{e}^{-\kappa \ell_{ij}}}{2\kappa}$$

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The eigenfunction corresponding to the ground state, i.e. c for which the minimum is reached can be chosen *strictly positive*; this follows from the fact that the semigroup $\{\mathrm{e}^{-t\Gamma_{\alpha,Y}(\kappa)} :\ t \geq 0\}$ is positivity improving

Proof by Krein's formula, continued

This means, in particular, that we have

$$\mu_0(\alpha, Y; \kappa) = \min_{|c|=1, c>0} \big(c, \Gamma_{\alpha,Y}(\kappa)c\big)$$

Proof by Krein's formula, continued

This means, in particular, that we have

$$\mu_0(\alpha, Y; \kappa) = \min_{|c|=1, c>0} \big(c, \Gamma_{\alpha,Y}(\kappa)c\big)$$

Take now two configurations, (α, Y) and $(\alpha, \tilde{Y})$ such that $\ell_{ij} \le \tilde{\ell}_{ij}$ and the inequality is strict for at least one pair (i,j). For a fixed $c > 0$ we have $\big(c, \Gamma_{\alpha,Y}(\kappa)c\big) < \Big(c, \Gamma_{\alpha,\tilde{Y}}(\kappa)c\Big)$, and consequently, taking a minimum overs all such c's we get

$$\mu_0(\alpha, Y; \kappa) < \mu_0(\alpha, \tilde{Y}; \kappa)$$

for all κ with the obvious implication for the ground state of $-\Delta_{\alpha,Y}$; the sharp inequality holds due to the fact that there is a c for which the minimum is attained. $\square$

Quantum graphs

More complicated “1D” problems one can find in *quantum graphs*. Consider such a graph Γ consisting of *vertices*, $\mathcal{V} = \{\mathcal{X}_j : j \in I\}$, and *edges* of two categories, *finite*, $\mathcal{L} = \{\mathcal{L}_{jn} : (\mathcal{X}_j, \mathcal{X}_n)$ with $(j, n) \in I_{\mathcal{L}} \subset I \times I\}$, and *infinite*, $\mathcal{L}_\infty = \{\mathcal{L}_{k\infty} : k \in I_{\mathcal{C}}\}$. We regard Γ as a configuration space of a quantum system with the Hilbert space

$$\mathcal{H} = \bigoplus_{j \in I_{\mathcal{L}}} L^2([0, l_j]) \oplus \bigoplus_{k \in I_{\mathcal{C}}} L^2([0, \infty))$$

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The Hamiltonian acts as $-\mathrm{d}^2/\mathrm{d}x^2$ on each edge; to make it self-adjoint s-a, general boundary conditions

$$(U_j - I)\Psi_j + i(U_j + I)\Psi'_j = 0$$

with unitary matrices U_j have to be imposed at the vertices $\mathcal{X}_j$, where Ψ_j and Ψ'_j are vectors of boundary values

Assumptions

We will be interested in the following particular situation:

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$$\psi_{j,i}(0) = \psi_{j,k}(0) =: \psi_j(0)\,, j,k = 1,\dots,n_j\,, \quad \sum_{i=1}^{n_j} \psi'_{j,i}(0) = \alpha_j \psi_j(0)\,,$$

where $n_j = \deg \mathcal{X}_j$ and edges are parametrized so that $x = 0$ corresponds to the vertex. In particular, we have Robin condition, $\psi'_j(l_j) + \alpha_j \psi_j(l_j) = 0$, at “free endpoints”

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- all the couplings involved are *non-repulsive*, $\alpha_j \le 0$ for all $j \in I$, and at least one of them is *attractive*, $\alpha_{j_0} < 0$ for some $j_0 \in I$

Existence of negative spectrum

The quadratic form of H can be then written as

$$q[\Psi] = \sum_{j\in I_{\mathcal{L}}} \int_0^{l_j} |\psi_j'(x)|^2\,\mathrm{d}x + \sum_{k\in I_{\mathcal{C}}} \int_{\mathbb{R}_+} |\psi_k'(x)|^2\,\mathrm{d}x + \sum_{i\in I} \alpha_i |\psi_i(0)|^2$$

being defined on L^2 functions which are $W^{1,2}$ on the graph edges and continuous at the vertices

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Proof: If $I_{\mathcal{C}} = \emptyset$ we take $\Psi = c$ on Γ which belongs to $\mathrm{Dom}[q]$ because $|\Gamma| < \infty$; we get $q[\Psi] \le \alpha_{j_0} |c|^2$. If $I_{\mathcal{C}} \ne \emptyset$, we take $\Psi = c$ on the internal part of the graph and $\psi_k(x) = c\,\mathrm{e}^{-\kappa x}$ on each external semiinfinite edge, obtaining

$$q[\Psi] \le \left(\alpha_{j_0} + \frac{1}{2}\kappa \sharp I_{\mathcal{C}} \right) |c|^2$$

which can be made < 0 by choosing κ small enough. $\square$

Existence of ground state

Theorem [E-Jex'12]: In addition, let Γ be connected, then $\lambda_0 = \inf \sigma(H)$ is a simple isolated eigenvalue. The corresponding eigenfunction $\Psi^{(0)}$ can be chosen strictly positive on Γ being convex on each edge

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Proof: $\sigma(H)$ is discrete if $I_{\mathcal{C}} = \emptyset$, otherwise one checks easily using Krein's formula that $\sigma_{\mathrm{ess}}(H) = \mathbb{R}_+$ and $\sigma_{\mathrm{disc}}(H) \subset \mathbb{R}_-$ is finite; by the previous result it is non-empty.

The ground state positivity follows, for instance, from a quantum-graph modification of Courant theorem [Band et al.'11]. The ef being positive and its component $\psi_j^{(0)}$ at the jth edge twice differentiable away of the vertices, we have $(\psi_j^{(0)})'' = -\lambda_0 \psi_j^{(0)} > 0$, which means the convexity. $\square$

Ground state edge indices

In fact, we know more. Writing $\lambda_0 = -\kappa^2$ we see that the ef component on each edge is a linear combination of $\mathrm{e}^{\kappa x}$ and $\mathrm{e}^{-\kappa x}$. Since we are free to choose the edge orientation, each component has one of the following three forms,

$$\psi_j^{(0)}(x) = \begin{cases} c_j \cosh \kappa(x+d_j) & \dots \quad d_j \in \mathbb{R} \\ c_j\, e^{\pm\kappa(x+d_j)} & \dots \quad d_j \in \mathbb{R} \\ c_j \sinh \kappa(x+d_j) & \dots \quad x+d_j > 0 \end{cases}$$

where c_j is a positive constant.

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where c_j is a positive constant. For further purposes we introduce *edge index*

$$\sigma_j := \begin{cases} +1 & \dots & \psi_j^{(0)}(x) = c_j \cosh \kappa(x+d_j) \\ 0 & \dots & \psi_j^{(0)}(x) = c_j\, e^{\pm\kappa(x+d_j)} \\ -1 & \dots & \psi_j^{(0)}(x) = c_j \sinh \kappa(x+d_j) \end{cases}$$

Ground state monotonicity

Given Γ and $\tilde{\Gamma}$ with the same topology differing possibly by inner edge lengths, we say they belong to the same *ground-state class* in the indices are the same for them and all interpolating graphs.

For connected graphs we have then the following result:

Theorem [E-Jex'12]: Under the stated assumptions, consider graphs Γ and $\tilde{\Gamma}$ of the same ground-state class. Let H and $\tilde{H}$ be the corresponding Hamiltonians with the same couplings in the respective vertices, and λ_0 and $\tilde{\lambda}_0$ the corresponding ground-state eigenvalues. Suppose that $\sigma_j \tilde{l}_j \leq \sigma_j l_j$ holds all $j \in I_{\mathcal{L}}$ such that $|\sigma_j| = 1$ and $\tilde{l}_j = l_j$ if $\sigma_j = 0$, then $\tilde{\lambda}_0 \leq \lambda_0$; the inequality is sharp if $\sigma_j \tilde{l}_j < \sigma_j l_j$ holds for at least one $j \in I_{\mathcal{L}}$.

Proof by a scaling argument

It is sufficient to consider length change of a single edge and prove the claim *locally*. We pick a segment in the interior of the a fixed edge and scale it by factor ξ *being less than one in case of shrinking and larger than one otherwise*

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We have to find $\Psi \in L^2(\tilde{\Gamma})$ such that the Rayleigh quotient on $\tilde{\Gamma}$ satisfies

$$\frac{\tilde{q}[\Psi]}{\|\Psi\|^2} < \lambda_0$$

for $\xi < 1$ if $\sigma_j = 1$ and $\xi > 1$ if $\sigma_j = -1$. We construct such a trial function $\tilde{\Psi}^{(0)}$ putting $\tilde{\Psi}^{(0)}(x) = \Psi^{(0)}(x)$ for $x \in \Gamma_J$, while the jth component on $\tilde{J}$ is obtained by scaling

$$\tilde{\psi}_j^{(0)}(\tilde{a} + \xi y) = \psi_j^{(0)}(a + y) \quad \text{for} \quad 0 \le y \le |J|$$

Proof by a scaling argument, continued

The Rayleigh quotient can be then easily rewritten as

$$\frac{\tilde{q}[\tilde{\Psi}^{(0)}]}{\|\tilde{\Psi}^{(0)}\|^2} = \frac{a+b\xi^{-1}}{c+d\xi} =: f(\xi)\,,$$

where

$$a := q_{\Gamma_J}[\Psi^{(0)}]\,, \quad b := \int_J |(\psi_j^{(0)})'(x)|^2\,\mathrm{d}x$$

and c, d are the parts of the squared norm of $\Psi^{(0)}$ corresponding to $\Gamma \setminus J$ and J, respectively

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Check that $\sigma_j f'(1) = -\sigma_j(bc + 2bd + ad)(c+d)^{-2} > 0$.

Choosing $\|\Psi^{(0)}\| = 1$, we have $c + d = 1$ and $a + b = \lambda_0$, hence the property to be checked is $-\sigma_j(\lambda_0 d + b) > 0$, or more explicitly

$$-\sigma_j \left(\lambda_0\|\psi_j^{(0)}\|_J^2 + \|(\psi_j^{(0)})'\|_J^2\right) > 0$$

Proof by a scaling argument, continued

Using $\lambda_0 = -\kappa^2$ we find for $\sigma_j = 1$

$$\int_J |(\psi_j^{(0)})'(x)|^2 \,\mathrm{d}x = c_j^2\kappa^2 \int_J (\sinh \kappa x)^2 \,\mathrm{d}x < c_j^2\kappa^2 \int_J (\cosh \kappa x)^2 \,\mathrm{d}x$$
$$= -\lambda_0 \int_J |\psi_j^{(0)}(x)|^2 \,\mathrm{d}x$$

and the opposite inequality for $\sigma_j = -1$ where the roles of hyperbolic sine and cosine are interchanged, which is what we have set out to prove. $\square$

Chain graphs

Corollary: Under our assumptions, suppose that *graph* Γ *has no branchings*, i.e. the degree of no vertex exceeds two. Then the index of any edge is non-negative being equal to one for any internal edge, hence *a length increase of any internal edge moves the ground-state energy up.*

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Proof: By assumption Γ is a chain, either a loop or an open chain. Consider the latter possibility; the former can be dealt with using Krein's formula similarly as above

Obviously it is impossible to have all the indices negative; the question is whether one can have a $\sinh$-type solution at some position within the chain

Proof, continued

Then wavefunction components with different indices have to match somewhere. Parametrize the chain by a single variable x choosing $x = 0$ for the vertex in question. Let the ground-state eigenfunction be $\psi_j(x) = \cosh\kappa(d_1 - x)$ for $x < 0$ and $\psi_{j+1}(x) = c\,\sinh\kappa(d_2 \mp x)$ for $x > 0$. They are coupled by an *attractive* δ interaction, hence c is determined by the continuity requirement and $\psi'_{j+1}(0+) - \psi'_j(0-)$ must be *negative*; recall that $\psi_j(0-) = \psi_{j+1}(0+) > 0$

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However, this expression equals $\mp\kappa \cosh \kappa(d_1 \pm d_2)/ \sinh \kappa d_2$, hence the needed match is impossible for a $\sinh$ solution decreasing towards the vertex. The same is true for the opposite order of the two solutions, and in a similar way one can check that a negative-index edge cannot neighbour with a semiinfinite one. $\square$

Branched graphs

This is no longer true for graphs with branchings as one can illustrate on a *simple example*

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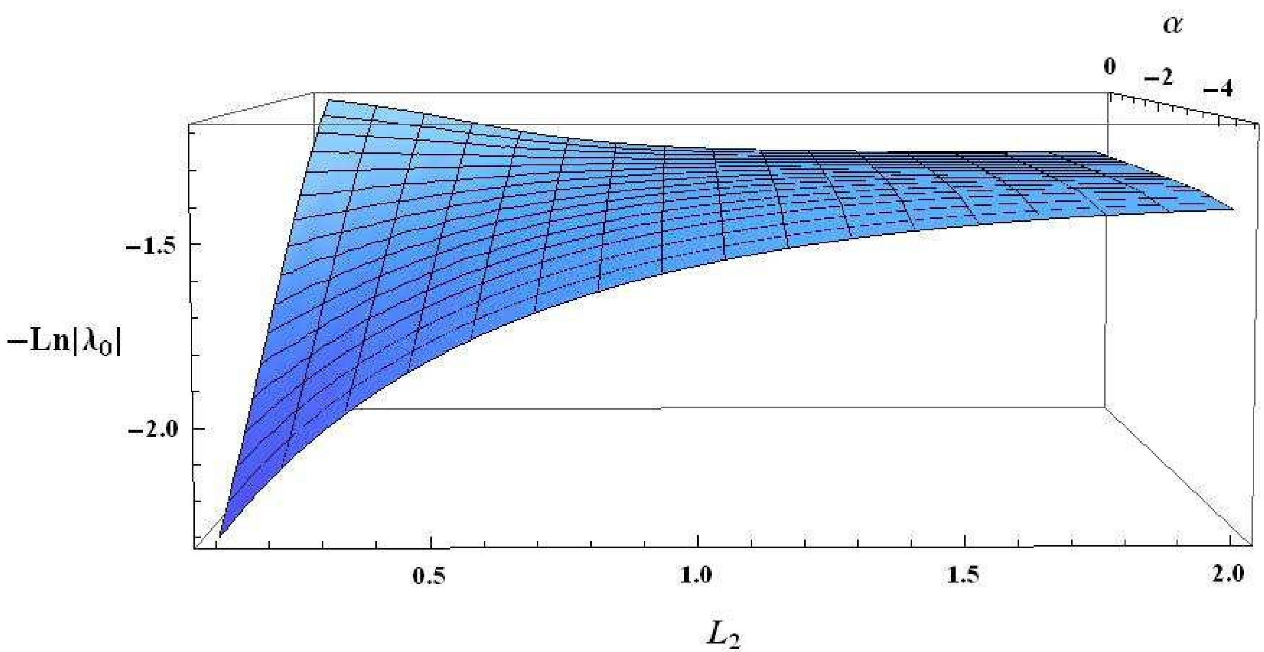

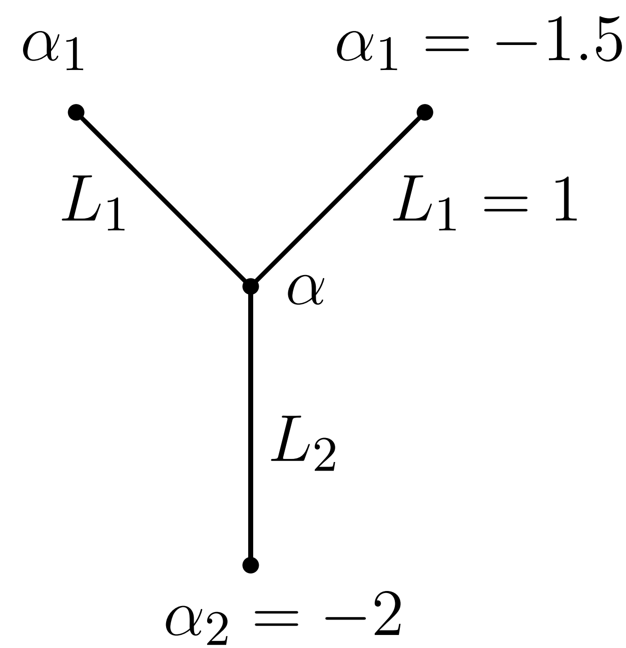

We see *different regimes* with transition at $\alpha_{\text{crit}} \approx -1.09088$

Point interactions in $\mathbb{R}^d$, $d = 2, 3$

Consider the Hamiltonians $-\Delta_{\alpha, Y_1}$ mentioned in the introduction with a finite set Y. The problem is dimension dependent: the ground state exists *for all* $\alpha \in \mathbb{R}^N$ *if* $d = 2$ while *for* $d = 3$ *we have to assume that* α_j*'s are below a critical value*. In analogy with the 1D case we have

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Theorem: Let $\sharp Y_1 = \sharp Y_2$ and $y_{1,i} - y_{1,j} \le y_{2,i} - y_{2,j}$ for all i, j with $y_{1,i} - y_{1,j} < y_{2,i} - y_{2,j}$ holding for at least one pair of i, j, then we have $\min \sigma(-\Delta_{\alpha,Y_1}) < \min \sigma(-\Delta_{\alpha,Y_2})$

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Proof: We employ Krein's formula approach again. The above proof was based on the fact that Green's function is *decreasing with the distance between the points.* This is true in $d = 2, 3$ too, hence the argument can be modified to the present case $\square$

Bracketing argument

We can again use bracketing. Now we need *no derivative assumption*, however, one has to establish instead existence of *“Neumann curve”*. Sometimes it is easy

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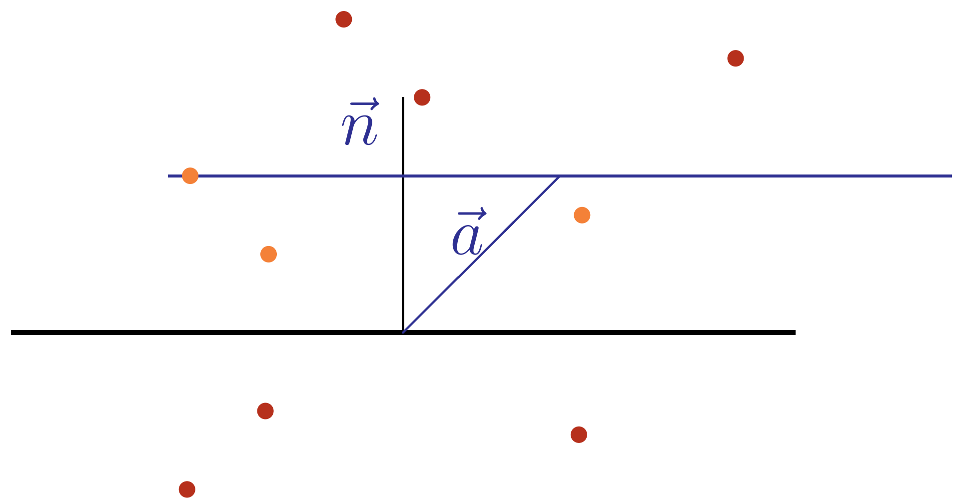
Example:



Call $H_{\vec{a}}$ the operator with "a half" of point interaction shifted; then if $\theta(\vec{a},\vec{n}) \leq \frac{\pi}{2}$ we have

$$\inf \sigma(H_{\vec{a}}) \geq \inf \sigma(H_{\vec{0}})$$

A generalization: leaky graphs

The results extend to singular Schrödinger operators

$$H_{\mu,\Gamma} = -\Delta - \mu(x)\delta(x-\Gamma)$$

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Using it one can prove ground-state monotonicity, e.g., for

- shifting curves Γ_1, Γ_2 *pointwise* towards each other
- "crumpling" a given curve Γ

Open questions

The above results inspire a host of questions, e.g.

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- *Regular-potential analogues* of the results described here, etc., etc.

The talk was based on

[E05a] P.E.: An isoperimetric problem for point interactions, *J. Phys. A: Math. Gen.* **A38** (2005), 4795-4802

[E05b] P.E.: Necklaces with interacting beads: isoperimetric problems, *Proceedings of the "International Conference on Differential Equations and Mathematical Physics" (Birmingham 2005),* AMS "Contemporary Mathematics" Series, vol. 412, Providence, R.I., 2003; pp. 141–149.

[EHL05] P.E., E. Harrell, M. Loss: Global mean-chord inequalities with application to isoperimetric problems, *Lett.Math.Phys.* **75** (2006), 225–233; addendum **77** (2006), 219

[EM08] P.E., A. Mantile: On the optimization of the principal eigenvalue for single-centre point-interaction operators in a bounded region, *J. Phys. A: Math. Gen.* **A41** (2008), 065305

[EJ12] P.E., I. Jex: On the ground state of quantum graphs with attractive δ-coupling, *Phys. Lett.* **A376** (2012), 713–717.

Thank you for your attention!