Isoperimetric problems for point sources and inequalities for loop chords

Pavel Exner

exner@ujf.cas.cz

Department of Theoretical Physics, NPI, Czech Academy of Sciences

and Doppler Institute, Czech Technical University

Talk overview

- *Motivation:* some classical and less classical isoperimetric problems for Schrödinger operators

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- *Another motivation* coming from electrostatics: charged necklaces

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- *Regular polygons* as local extrema for polymer loops and charged necklaces
- *Global maximizer:* a sufficient condition
- *Summary and outlook*

Motivation

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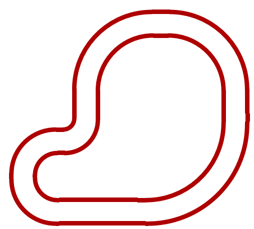
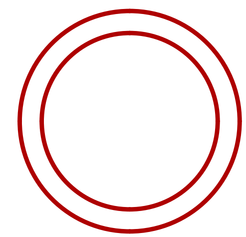
similarly *a ball* is a minimizer for a compact $M \subset \mathbb{R}^d,\ d \geq 3$

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

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

Notice that topology is important

If M is not simply connected, rotational symmetry may again lead to an extremum but its nature can be different. Recall a *a strip of fixed length and width* [E.-Harrell-Loss'99]

ground state of  $<$ ground state of 

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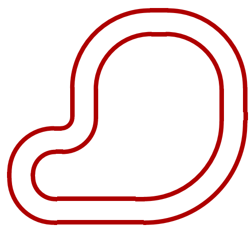
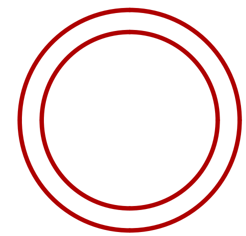
ground state of  $<$ ground state of 

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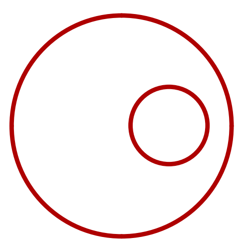
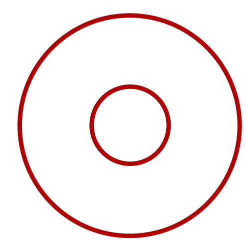
Another example is a *circular obstacle in circular cavity* [Harrell-Kröger-Kurata'01]

ground state of  $<$ ground state of 

whenever the obstacle is off center

Singular Schrödinger operators

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$$-\Delta + \tilde{\alpha} \sum_{j=1}^{N} \delta(x - y_j) \quad \text{in } L^2(\mathbb{R}^d)\,,\; d = 2, 3\,,$$

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where the y_j's are vertices of an *equilateral polygon* $\mathcal{P}_N$

In the same vein one can analyze an attractive δ potential supported by a *closed loop Γ of fixed length*, i.e.

$$-\Delta - \alpha\delta(x - \Gamma) \quad \text{in } L^2(\mathbb{R}^2)$$

Polymer loops

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It is an extension of the "discrete" problem to a more general class of curves: we take a closed loop Γ and consider a class of singular Schrödinger operators in $L^2(\mathbb{R}^d),\ d=2,3,$ given formally by the expression

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

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

Charged necklaces

We will consider at the same time another problem which concerns a *charged necklace*. It comes from *classical electrostatics* and at a glance it has a little in common with the quantum mechanical question posed above

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We are going to show that both these problems reduce essentially to *the same geometric question*

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

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

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

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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 local maximum

To begin with, let us formulate the assumptions:

Γ is a continuous, piecewise C^1 function, $[0,L] \to \mathbb{R}^d$, such that $\Gamma(0) = \Gamma(L)$ and $|\dot\Gamma(s)| = 1$ holds for any $s \in [0,L]$

In fact that we consider $\mathbb{R} \to \mathbb{R}^d \; (\mathrm{mod}\, L)$, i.e. $y_j = y_{j(\mathrm{mod}\, N)}$; an argument shift means a trivial reparametrization.

Spectra of $-\Delta_{\alpha,Y_\Gamma}$ and $-\Delta_{\alpha,Y_{\Gamma'}}$ corresponding Euclidean related Γ and Γ' are the same; speaking about curves we have naturally in mind such equivalence classes

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Spectra of $-\Delta_{\alpha, Y_\Gamma}$ and $-\Delta_{\alpha, Y_{\Gamma'}}$ corresponding Euclidean related Γ and Γ' are the same; speaking about curves we have naturally in mind such equivalence classes

Theorem: Under the stated assumptions, the (nontrivial) ground state $\epsilon_1(\alpha, Y_\Gamma)$ is for fixed α and $L > 0$ *locally sharply maximized* by a regular planar polygon, $\Gamma = \tilde{\mathcal{P}}_N$.

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

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

holds *for all* $\kappa > 0$ and $\Gamma \neq \tilde{\mathcal{P}}_N$.

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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

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

where ν_n is the number of the appropriate chords

Geometric reformulation, continued

It is easy to see that

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

since for an even N one has to prevent double counting

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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 purely geometric

More general chord inequalities

Recall that for a loop $\Gamma :\ [0, L] \to \mathbb{R}^2$ we have introduced

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

For fixed $L > 0$, N and $m = 1, \ldots, [\frac{1}{2}N]$ 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 $\tilde{\mathcal{P}}_N$

Simple observations

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- By *scaling* one can put, for instance, the loop length $L = 2\pi$ without loss of generality
- 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

Elementary properties

Using convexity of $x \mapsto x^\alpha$ in $(0, \infty)$ for $\alpha > 1$ we get

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

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Conjecture: We expect the above inequalities to be valid for any $p \leq 2$, without substantial restrictions to the regularity of Γ

Local validity of $D^1_{L,N}(m)$

We are looking for constrained local maxima of the function

$$f_m: \; f_m(y_1, \ldots, y_N) = \frac{1}{N} \sum_{i=1}^{N} |y_i - y_{i+m}|$$

with $g_i(y_1, \ldots, y_n) := \frac{L}{N} - |y_i - y_{i+1}| \geq 0,\; i = 1, \ldots, N$. There are in fact $(N-2)(d-1)-1$ independent variables because $2d-1$ parameters are related to Euclidean transformations

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Following the convention for inequality-type constraints we introduce *slack variables* z_r, $r = 1, \dots, N$, and Lagrange multipliers λ_r, $r = 1, \dots, N$, which determine

$$K_m(y_1, \dots, y_N, z_1, \dots, z_N) := f_m(y_1, \dots, y_N) + \sum_{r=1}^{N} \lambda_r \left(g_r(y_1, \dots, y_n) - z_r^2 \right)$$

Local validity, continued

It is straightforward to check that $\nabla_j K_m(y_1, \ldots, y_N)$ vanish for a regular planar polygon, with all the Lagrange multipliers taking the same value

$$\lambda = \frac{\sigma_m}{N \Upsilon_m} \quad \text{with} \quad \sigma_m := \frac{\sin^2 \frac{\pi m}{N}}{\sin^2 \frac{\pi}{N}}, \ \Upsilon_m := \ell^{-1} |\tilde{y}_j - \tilde{y}_{j \pm m}|$$

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At the same time, one requires vanishing of the derivatives

$$\partial_{z_j} K_m = 2 \lambda_j z_j \,, \quad j = 1, \dots, N,$$

which means that at the extremum all the slack variables vanish, $z_j = 0$. This is not surprising; one expects critical points of f_m to be reached under given constraints with the neighbour distances maximal, i.e. for a polygon

Local validity, continued

Negative definiteness of the Hessian needs more computation. A simple estimate then shows that it is sufficient to establish negative definiteness of the form

$$\xi \mapsto S_m[\xi] := \sum_j \left\{ |\xi_j - \xi_{j+m}|^2 - \sigma_m |\xi_j - \xi_{j+1}|^2 \right\}$$

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The two parts can be simultaneously diagonalized; using their ev's one rewrites the condition as the inequality

$$U_{m-1}\left(\cos\frac{\pi}{N}\right) > \left| U_{m-1}\left(\cos\frac{\pi r}{N}\right) \right|, \; r = 2, \ldots, m-1 \,,$$

for Chebyshev polynomials of the second kind which can be checked directly. *This proves the above theorem*

Application to charged necklaces

Theorem: Under the stated assumptions, the Coulomb energy of a charged necklace is locally sharply minimized by a regular planar polygon, $\Gamma = \tilde{\mathcal{P}}_N$

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Proof: For a given nonzero charge q of each “bead” the potential energy equals

$$q^2 \sum_{j \neq k} |y_j - y_k|^{-1} = q^2 \sum_{m=1}^{\left[\frac{1}{2}N\right]} \frac{\nu_m}{N} \sum_{n=1}^{N} |y_{n+m} - y_n|^{-1},$$

and since the inequality $D^1_{L,N}(m)$ implies $D^{-1}_{L,N}(m)$, the sum of all repulsion-energy terms is locally sharply minimized by $\tilde{\mathcal{P}}_N$. $\square$

Is $D^2_{L,N}(m)$ globally valid?

Try to adapt the idea of [EHL'05] in the "discrete" case. 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 $c_{-n} = \bar{c}_n$. Notice that the assumption $c_0 = 0$ can be always satisfied by a choice of the coordinate system.

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It is convenient to assume $\Gamma \in C^2$; the validity of $D^2_{L,N}(m)$ can be extended by means of Weierstrass theorem and continuity of the functions involved. Then the derivative of Γ is a sum of the uniformly convergent Fourier series

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

Global validity, continued

The arc-length parametrization, $|\dot{\Gamma}(s)| = 1$, gives

$$2\pi = \int_0^{2\pi} |\dot{\Gamma}(s)|^2 \,\mathrm{d}s = \int_0^{2\pi} \sum_{0\neq l\in\mathbb{Z}} \sum_{0\neq n\in\mathbb{Z}} nl\, c_l^* \cdot c_n \,\mathrm{e}^{i(n-l)s} \,\mathrm{d}s\,,$$

where $c_l^* = (\bar{c}_{l,1}, \ldots, \bar{c}_{l,d})$, or equivalently, the condition

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

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

Global validity, 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

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

Global validity, 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

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

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$A^{(N,m)}$ is obviously bounded because its Hilbert-Schmidt norm is finite. Since $\|d\| = 1$ by construction, we arrive at the following conclusion:

Proposition: The inequality $D_{L,N}^2(m)$, and thus also $D_{L,N}^{\pm p}(m)$ with $p \leq 2$, for fixed values of $N = 2, 3, \dots$ and $m = 1, \dots, \left[\frac{1}{2}N\right]$ is valid provided the norm of the operator $A^{(N,m)}$ does not exceed $\left(\frac{\pi \sin\frac{\pi m}{N}}{N \sin\frac{\pi}{N}}\right)^2$.

Remarks

- The “continuous” case 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*

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- In the "continuous" case one uses Parseval relation and the integral analogue of $\sum_{i=1}^{N} |y_i - y_{i+m}|^2$ is naturally *invariant w.r.t. shifts in the arc-length parametrization*. This is not true here; the shift $s \to s + s_0$ is equivalent to the replacement of c_j by $c_j \mathrm{e}^{is_0}$, which changes in general the expression due to the presence of the off-diagonal terms

Summary and outlook

- In contrast to the “continuous” case the argument giving the global solution is more difficult to be completed, but *it can be done* – *a work in progress*

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- *Open question:* to find extrema in situations *without a built-in symmetry*, i.e. with different couplings or source spacing. This problem is no longer purely geometric

Summary and outlook

- In contrast to the “continuous” case the argument giving the global solution is more difficult to be completed, but *it can be done* – *a work in progress*
- *Open question:* to find extrema in situations *without a built-in symmetry*, i.e. with different couplings or source spacing. This problem is no longer purely geometric
- *Another open question:* to find *higher-dimensional analogues* of the inequalities discussed here

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.: An isoperimetric problem for leaky loops and related mean-chord inequalities, *J. Math. Phys.* **46** (2005), 062105

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