Spectral properties of some quantum systems with wires in $\mathbb{R}^3$

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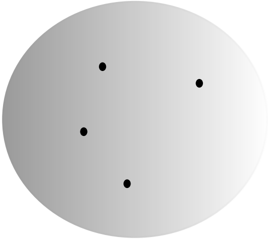
P. Exner, S. Kondej, Spectral optimization for strongly singular Schrödinger operators with a star-shaped interaction, 2019
S. Kondej, Bound states asymptotics in the system with quantum wires in $\mathbb{R}^3$, 2022

Auxiliary: Thomson problem (1904)



electrons on sphere

Electrons localized at $x_1, ..., x_N$.

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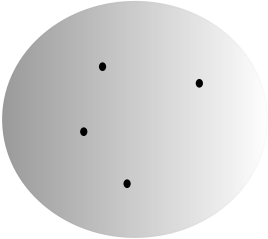

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- The electrostatic interaction energy between a pair of electrons of equal charges

$$U = k\frac{e^2}{r_{ij}}\,, \quad r_{ij} = |x_i - x_j|\,, \quad x_i \in S^2\,.$$

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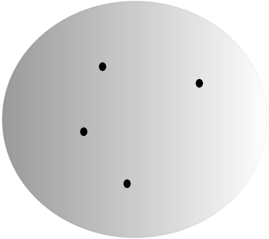

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- The total electrostatic potential energy of each N-electron ($k = e = 1$)

$$U(N) = \sum_{i<j} \frac{1}{r_{ij}} .$$

Formulation of problem.

Determine the minimum potential energy configuration of N electrons constrained to the surface of a unit sphere that repel each other with a force given by Coulomb's law. Find a configuration of electrons for which

$$U(N) = \sum_{i<j} \frac{1}{r_{ij}} .$$

assumes minimum.

Generalized Thomson model

Consider a continuous function $f : [0, 4) \to [0, \infty)$. Given a finite subset $\mathcal{C}$ of points residing on the unit sphere S^2 define the potential energy of $\mathcal{C}$ to be

$$\sum_{x_i, x_j \in \mathcal{C}, i \neq j} f(|x_i - x_j|^2) \,. \tag{1}$$

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Completely monotonic function

f is completely monotonic if

$$(-1)^k f^{(k)}(x) \geq 0 \,, \, \forall x \in I \,, \; \forall k \geq 0 \,.$$

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Cohn – Kumar Theorem

If f strictly completely monotonic, then (1) achieves unique minimum for $\mathcal{C}$ determining the sharp configuration.

Sharp agreement

Consider N points $\{x_i\}_{i=1}^N$ placed on a unit sphere S^2. They are said to form an *M-spherical design* if for any polynomial function $S^2 \ni x \mapsto p(x)$ of total degree at most M its mean over $\{x_i\}$ coincides with the mean over the sphere,

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

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Suppose further that m denotes the number of the different values of inner product between the points, then $\{x_i\}_{i=1}^N$ is called a *sharp configuration* if it is $2m-1$ spherical design.

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Rigorously identified sharp configurations.

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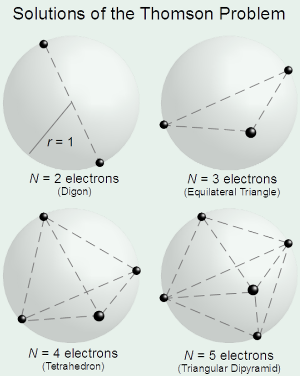
7th Smale's problem.

For the remaining N the problem is still open.
Thomson problem belongs to the Smale's problems list of eighteen unsolved problems in mathematics (proposed by Steve Smale in 1998).

Configuration for $N = 2, 3, 4, 5$



Thomson problem solutions vs Platonic solids

Platonic solid - regular, convex polyhedron, constructed by congruent (identical in shape and size) regular (all angles equal and all sides equal) polygonal faces with the same number of faces meeting at each vertex. Five solids meet these criteria:

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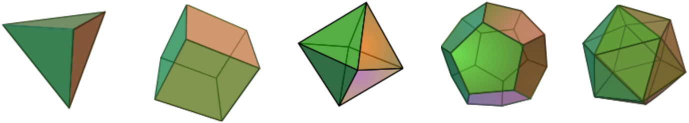

source: Wikipedia 1. Tetrahedron - Four faces (N=4)
2. Cube - Six faces (N=8)
3. Octahedron - Eight faces (N=6)
4. Dodecahedron - Twelve faces (N=20)
5. Icosahedron Twenty faces (N=12)

Thomson problem versus Platonic solids

$N = 4\,,6\,,12$

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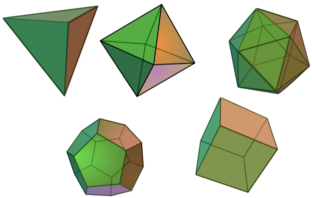

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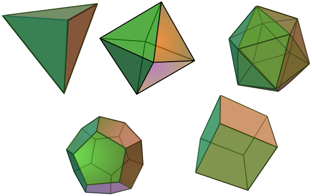


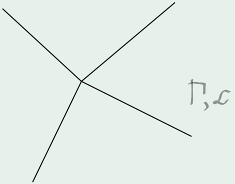
source: Wikipedia

$N = 8\,,N = 20$

Numerical solutions of Thomson problem for $N = 8\,,20$ are *not the regular convex polyhedral configurations of the remaining two Platonic solids*, whose faces are square and pentagonal, respectively.

Star shaped wire in $\mathbb{R}^3$

Formulation of problem: attractive star in $\mathbb{R}^3$. N- number of arms, L- length of each arm, α - coupling constant.



$\Gamma = \Gamma_1 \cup \Gamma_2 \cup \ldots \cup \Gamma_N$.

Hamiltonian

$$H_{\alpha,\Gamma} = \text{"} -\Delta + \alpha\delta(x - \Gamma)\text{"} \, . \tag{2}$$

Self-adjoint realization of $H_{\alpha,\Gamma}$

What is Hamiltonian with the star shape potential?

Operator

$$H_{\alpha,\Gamma} = " - \Delta + \alpha\delta(x - \Gamma)" \,.$$

is defined as a self-adjoint extension of

$$-\Delta|_{C_0^\infty(\mathbb{R}^3\setminus\Gamma)} \,.$$

$H_{\alpha,\Gamma} = " - \Delta + \alpha\delta(x - \Gamma)"$ is defined by means of the boundary conditions on Γ.

Attractivity of the potential

Two dimensional system with one point interaction $\mu_{\alpha,1} = -4e^{2(-2\pi\alpha+\psi(1))}$.

Boundary conditions, definition of Hamiltonian

Given $f \in W^{2,2}_{\mathrm{loc}}(\mathbb{R}^3 \setminus \Gamma)$ we pick a point $s \in \Gamma_i$ and its neighborhood (in the plane perp. to Γ_i at s) U_i of s disjoint with $\Gamma \setminus \Gamma_i$ and consider the restriction $f\restriction_{U_i}$ which is locally (in U_i) a distribution. Assume that

$$\Xi(f)(s) := -\lim_{\rho\to 0} \frac{1}{\ln\rho} f\restriction_{U_i}(s)\,,$$

$$\Omega(f)(s) := \lim_{\rho\to 0} \left[f\restriction_{U_i}(s) + \Xi(f)(s)\ln\rho \right]$$

exist almost everywhere in $(0, L)$ for any $i = 1, \dots, n$.

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Impose

$$2\pi\alpha\Xi(f) = \Omega(f)\,, \tag{4}$$

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$$H_{\alpha,\Gamma} f(x) = -\Delta f(x)\,, \;\; x \in \mathbb{R}^3 \setminus \Gamma\,.$$
$$D(H_{\alpha,\gamma}) := \{ f \in W^{2,2}_{\mathrm{loc}}(\mathbb{R}^3 \setminus \Gamma) \cap L^2(\mathbb{R}^3) \,:\, f \text{ satisfies } (4) \}$$

Spectral stage

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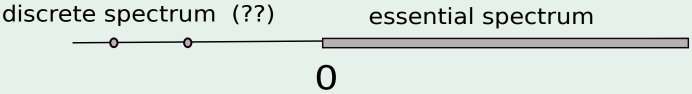

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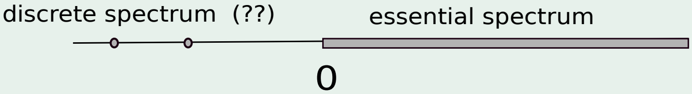

Analogy to well potential

For attractive interaction the ground state energy goes down if the attractive components approach and goes up if the attractive components go away.

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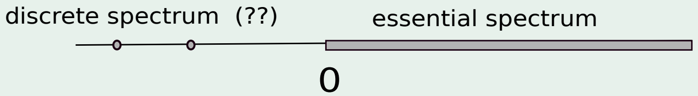

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Question 2. Main question:

For which configuration of arms the ground state energy is maximal?

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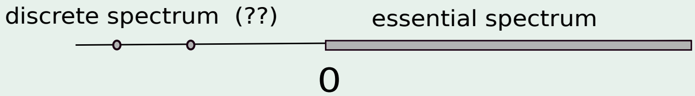

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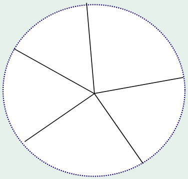
Does the discrete spectrum always exists for the star shape potential?

Two dimensional model: There exists always non empty discrete spectrum provided potential is attractive



P. Exner, V. Lotoreichik; 2018

The maximum the ground state energy is (uniquely) achieved for the regular polygon with angle $\frac{2\pi}{N}$.

Existence of discrete spectrum, cont.

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Three dimensional model; existence

Th. [P.Exner, SK, 2019] If $L > 2\pi\, \mathrm{e}^{2\pi\alpha - \psi(1)}$ then

$$\sigma_{\mathrm{disc}} \neq \emptyset\,,$$

whereΠ$-\,\psi(1) \approx 0.577$.

Existence of discrete spectrum, cont.

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Three dimensional model; non existence

Th. [P.Exner, SK, 2019] If

$$N \frac{1}{2\pi} \ln \frac{L}{4} + C_2 < \alpha\,, \tag{5}$$

where $C_2 = \sum_{i\neq j} \left(\frac{1}{4\pi} |\ln \phi_{ij}| + C_1 \right)$. Then

$$\sigma_{\mathrm{disc}} = \emptyset\,. \tag{6}$$

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$$\sigma_{\mathrm{disc}} = \emptyset\,. \tag{6}$$

In particular, if the star in too small/weak then (6) holds.

Optimization: Solution

Theorem. P. Exner, SK, 2019

Assume that $N \in \{2, 3, 4, 6, 12\}$. The lowest energy of $\hat{H}_{\alpha,\Gamma}$ assumes the unique maximum for Γ realizing the following configurations
$N = 2$ antipodal points,
$N = 3$ simplex with inner product $-1/2$,
$N = 4$ tetrahedron,
$N = 6$ octahedron,
$N = 12$ icosahedron,

Denote the above configuration as Σ.

Birman Schwinger principle poles of the resovent

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Resolvent

$$R_{\alpha,\Gamma}(z) = R(z) - \mathrm{R}_\Gamma(z)(\alpha - Q_{\kappa,\Gamma})^{-1}\check{\mathrm{R}}_\Gamma(z)\,, \quad z = -\kappa^2$$

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Birman-Schwinger principle

Rephrasing the investigation of $\sigma_{\mathrm{disc}}(H_{\alpha,\Gamma})$ as analysis of the operator $Q_{\kappa,\Gamma}$ can be expressed concisely as

$$f \in \ker(\alpha - Q_{\kappa,\Gamma}) \Leftrightarrow H_{\alpha,\Gamma} g_\kappa = -\kappa^2 g_\kappa \quad \text{where} \quad g_\kappa = G_\kappa * f\,. \tag{7}$$

Ideas of proofs.

We investigate $\ker(\alpha - Q_{\kappa,\Gamma})$. The operator-valued matrix

$$Q_{\kappa,\Gamma} := [T^{ij}_{\kappa,\Gamma}]^N_{i,j=1}\,, \quad \bigoplus_{i=1}^{N} L^2([0,L]) \tag{8}$$

$T^{ij}_{\kappa,\Gamma}:\ L^2([0,L]) \to L^2([0,L])$ are integral operators with the kernels

$$\begin{cases} T_{\kappa;s,t}(|\bar{\Gamma}_i - \bar{\Gamma}_j|^2) := G_\kappa(|\Gamma_i(s) - \Gamma_j(t)|) & \text{if } \ i \neq j \\ G^{\mathrm{reg}}_\kappa(\Gamma_i(s) - \Gamma_i(t)) & \text{if } \ i = j \end{cases} \tag{9}$$

where

$$G_\kappa(x,x') = \frac{1}{4\pi}\,\frac{{}^{-\kappa|x-x'|}}{|x-x'|}\,, \tag{10}$$

and G^{reg}_κ is the regularized kernel with the logarithmic singularity removed.

Ideas of proofs, cont.

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$$\ker(\alpha - Q_{\kappa,\Gamma})$$

$-\kappa^2$ corresponds to the eigenvalue of $H_{\alpha,\Gamma}$

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$$(f, T^{ii}_{\kappa,\Gamma} f) = (f, T^{ii}_{\kappa,\Sigma} f)$$

and, by Cohn – Kumar theorem:

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

Ideas of proofs, cont.

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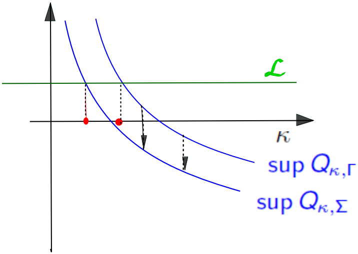
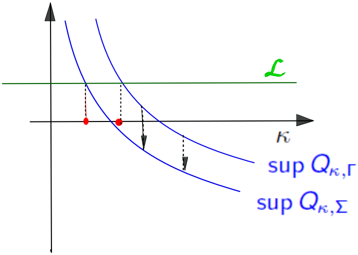
Find the configuration of $\{\Gamma_1, ..., \Gamma_N\}$ such that

$$\sup Q_{\kappa,\Gamma}$$

assumes minimum.

Ideas of proofs, cont.

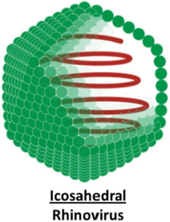




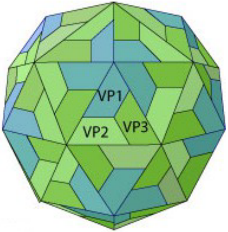
$$
\begin{aligned}
& \sup Q_{\kappa,\Gamma} \geq (Q_{\kappa,\Gamma}\tilde{f},\tilde{f}) \\
\geq\ & \sum_{i,j\ i\neq j} \int_{L\times L} T_{\kappa;s,t}((|\bar{\Gamma}_i - \bar{\Gamma}_j|^2))f(s)f(t)\mathrm{d}s\mathrm{d}t + \sum_{i=1}^{N} (f_i, T^{ii}_{\kappa,\Gamma} f_i) \\
\geq\ & \sum_{i,j\ i\neq j} \int_{L\times L} T_{\kappa;s,t}((|\bar{\Sigma}_i - \bar{\Sigma}_j|^2))f(s)f(t)\mathrm{d}s\mathrm{d}t + \sum_{i=1}^{N} (f, T^{ii}_{\kappa,\Sigma} f) \\
=\ & \sup Q_{\kappa,\Sigma}\,.
\end{aligned}
$$

Icosahedral packings in virus shells

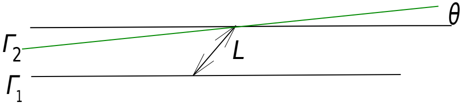
Source: Wikipedia



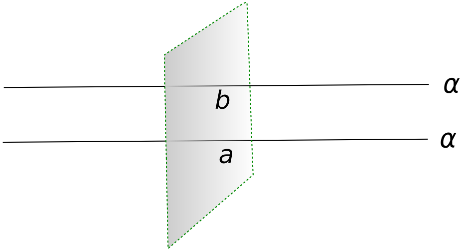
Source: MORGRIDGE INSTITUTE FOR RESEARCH OUTREACH EXPERIENCES



Small angle asymptotics



$$\Gamma_1(s) = (s, 0, 0) \, : \, \mathbb{R} \to \mathbb{R}^3 \,, \quad \Gamma_2(s) = (s\cos\theta, s\sin\theta, L) \, : \, \mathbb{R} \to \mathbb{R}^3 \,,$$

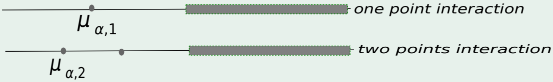


Point interaction in 2D

$$h_{\alpha,1} = -\Delta^{(2)} + \delta_\alpha(x-a) \,, \quad h_{\alpha,2} = -\Delta^{(2)} + \delta_\alpha(x-a) + \delta_\alpha(x-b)$$

Spectrum

Spectrum of $h_{\alpha,1}$ and $h_{\alpha,2}$



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

Essential spectrum of double line (parallel lines)

- For $\theta = 0$ we have

$$\sigma_{\mathrm{ess}}(H_{0,\alpha}) = [\mu_{\alpha,2}, \infty)\,.$$

Essential spectrum of double line (non parallel lines)

- For $\theta > 0$ we have

$$\sigma_{\mathrm{ess}}(H_{\theta,\alpha}) = [\mu_{\alpha,1}, \infty)\,, \qquad \mu_{\alpha,2} < \mu_{\alpha,1}$$

Properties of discrete spectrum

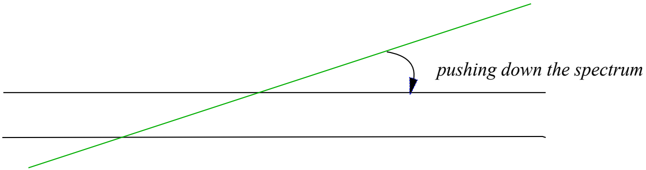
Discrete spectrum

- For $\theta > 0$ there exists discrete spectrum in $(\mu_{\alpha,2}\,,\mu_{\alpha,1})$.

Theorem, SK'22

The function $\theta \mapsto \inf\, \sigma(H_{\theta,\alpha})$ is increasing.

- It achieves maximum for $\theta = \frac{\pi}{2}$,
- It achieves minimum for $\theta = 0$.
- The whole discrete spectrum is contained in $(\mu_{\alpha,2}\,,\mu_{\alpha,1})$.



Counting function asymptotics

Theorem, SK'22

For $\theta \to 0$ the number of discrete spectrum points behaves as

$$N = \mathcal{O}(\theta^{-1})\,.$$

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We investigate $\ker(\alpha - Q_{\kappa,\Gamma})$. The operator-valued matrix

$$Q_{\kappa,\Gamma} := [T^{ij}_{\kappa,\Gamma}]^2_{i,j=1}\,,\quad \bigoplus_{i=1}^{2} L^2([0,L]) \tag{11}$$

$T^{ij}_{\kappa,\Gamma}\,:\; L^2(R) \to L^2(R)$ are integral operators with the kernels

$$\begin{cases} D_\theta := G_\kappa(|\Gamma_i(s) - \Gamma_j(t)|) & \text{if } \; i \neq j \\ G^{\mathrm{reg}}_\kappa(\Gamma_i(s) - \Gamma_i(t)) & \text{if } \; i = j \end{cases} \tag{12}$$

$$|\Gamma_i(s) - \Gamma_j(t)| = \sqrt{s^2 + t^2 + L^2 - 2st\cos\theta}\,.$$

We have

$$\|D_\theta\|^2_{\mathrm{HS}} = \int_{R\times R} |G_\kappa(|\Gamma_i(s) - \Gamma_j(t)|)|^2\,\mathrm{d}s\mathrm{d}t = \mathcal{O}(\theta^{-1})\,.$$

Bounds for the counting functions of $H_{\alpha,\theta}$

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Upper bound

$$\sharp\sigma_{ess}(H_{\alpha,\theta}) \leq \mathrm{const} + \mathrm{const} \cdot \|D_\theta\|^2_{HS} = \mathcal{O}(\theta^{-1})\,.$$

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Upper bound

$$\sharp\sigma_{ess}(H_{\alpha,\theta}) \leq \mathrm{const} + \mathrm{const}\cdot \|D_\theta\|_{HS}^2 = \mathcal{O}(\theta^{-1})\,.$$

Lower bound

Construction of $N = [\theta^{-1}]$ functions ϕ_λ

$$(H_{\alpha,\theta}\phi_\lambda, \phi_\lambda) - \mu_{1,\alpha}(\phi_\lambda, \phi_\lambda) < 0$$

Thank you for your attention