There is more in quantum mechanics

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What a mathematician can say here

When I was invited to give a talk here I thought what I can say without boring you with our ϵ's and δ's

I decided to show you some things a mathematician's eye may observe in quantum mechanics

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Indeed, is something can be called *a substance of modern material science* it is without any doubt quantum mechanics

Properties of materials we use are determined primarily by their atomic and molecular structure which is described by well-understood quantum mechanical equations

But all the same ...

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Than are dreamt of in your philosophy

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If an excuse is needed, I can quote [Bratelli-Robinson'79]:

... while the experimentalist might collect all his data between breakfast and lunch in a small cluttered laboratory, his theoretical colleagues interpret those interpret those results in term of isolated systems moving eternally in an infinitely extended space. The validity of such idealizations is the heart and soul of theoretical physics and has the same fundamental significance as the reproducibility of experimental data

Geometrically induced bound states

As the first example let me show that in some quantum systems *bending induces binding*

Consider a nonrelativistic quantum particle in a 2D or 3D infinite tube Ω of width d. Since values of physical constants will not be important, we put $\frac{\hbar^2}{2m} = 1$ so the Hamiltonian is

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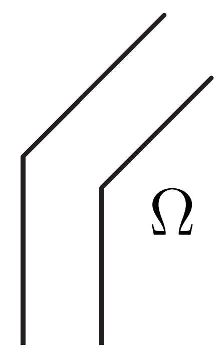
If Ω is straight, the spectrum is continuous starting at $\left(\frac{\pi}{d}\right)^2$

Let us now bend the tube. Note that from the classical-physics point of view not much changes: *the set of trapped trajectories has measure zero*



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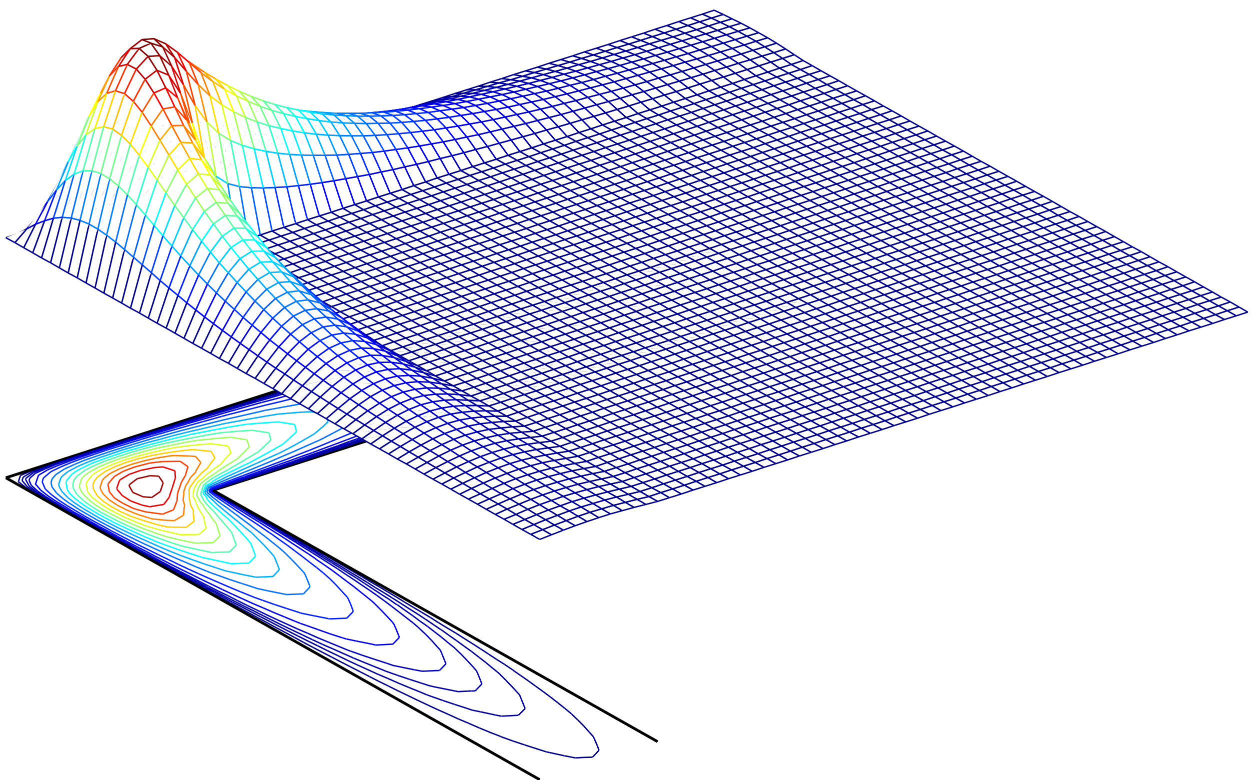
Theorem [E-Šeba-Šťovíček'89]: If Ω is *L–shaped*, there is exactly one eigenvalue $\lambda \equiv 0.929\ldots \left(\frac{\pi}{d}\right)^2$ of $-\Delta_D^\Omega$

L-shaped guide bound state



The ground-state eigenfunction $\psi(\vec{x})$ in an L-shaped guide

Binding mechanism

The best way to understand the effect is to consider a *smoothly bent tube* and to rewrite the Laplacian in the natural curvilinear coordinates (s, u) obtaining

$$H = -\partial_s (1 + u\kappa(s))^{-2} \partial_s - (\partial_u^2)_D + V_{\text{eff}}(s, u),$$

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If the *strip is thin* we get around the first threshold

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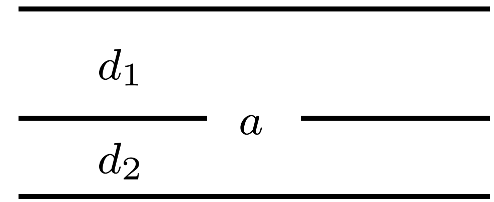
However, a variational argument [Goldstone-Jaffe'92, Duclos-E'95] shows that the *binding occurs for any* d

Laterally coupled QWG

There are other examples of "non-classical" bound states, e.g., in parallel waveguides *coupled through window in the common boundary*



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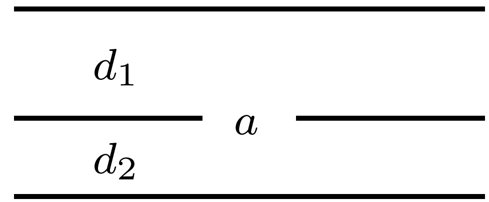
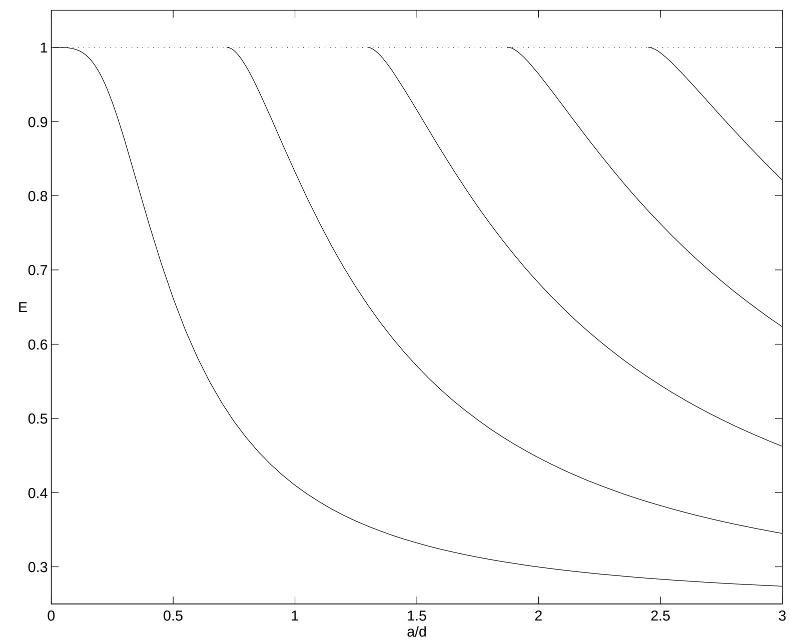
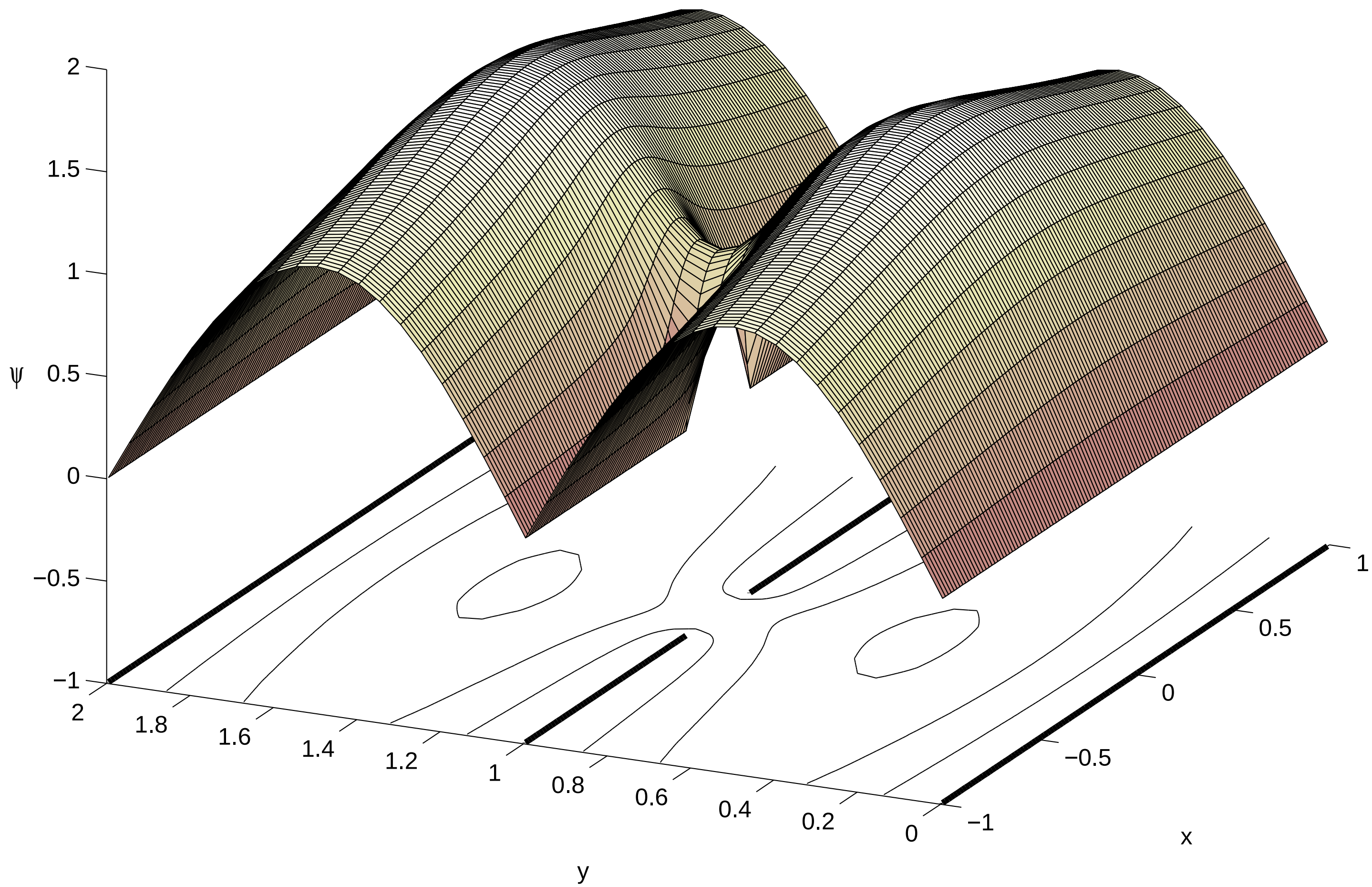


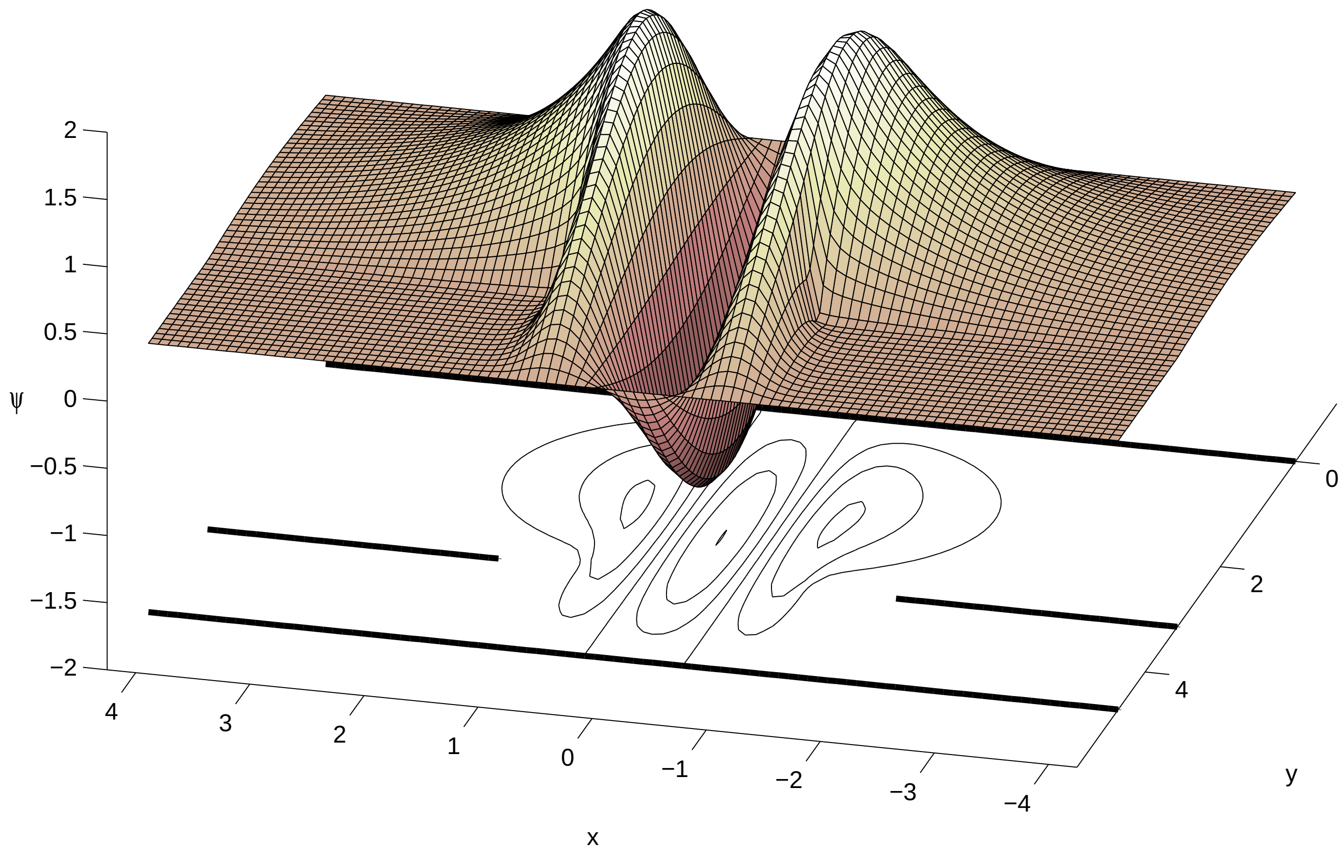
Theorem [E-Šeba-Tater-Vaněk'96]: $\sigma_{\text{disc}}(-\Delta_D^\Omega) \neq \emptyset$ holds for any window width $a > 0$. The number of bound states increases (roughly) linearly with a



Window-coupled ground state



A window-coupled excited state



One more example: scissor guide

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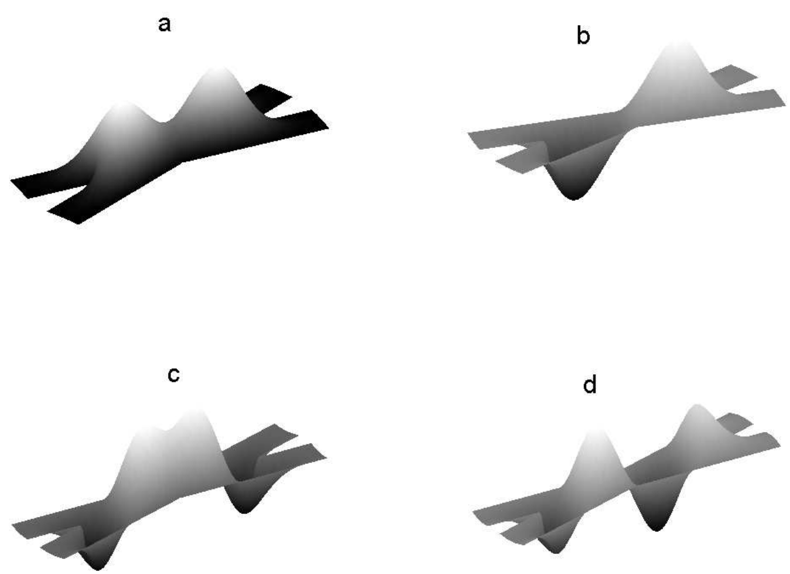
For $\theta = 30^{\circ}$, e.g., the crossed strips have *four bound states*



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- The same Helmholtz equation, $-\Delta_D^\Omega \psi = \lambda\psi$, can also be used to describe the TE$_{0m}$ modes in *flat electromagnetic waveguides*. Using this observation, the above conclusions were *tested experimentally* is microwave systems [Londergan-Carini-Murdock'99]

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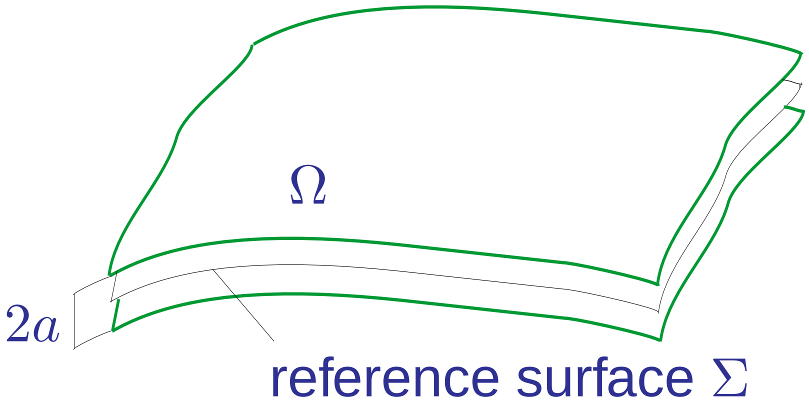
- A caveat: Not every geometrically induced coupling is attractive. For instance, *twisting* of a non-circular tube gives rise to an effective *repulsive interaction*, cf. [Ekholm-Kovařík-Krejčiřík'08]

Binding in curved layers



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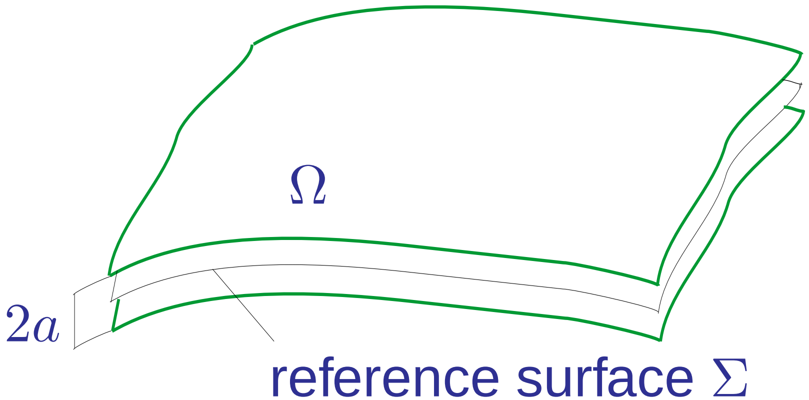

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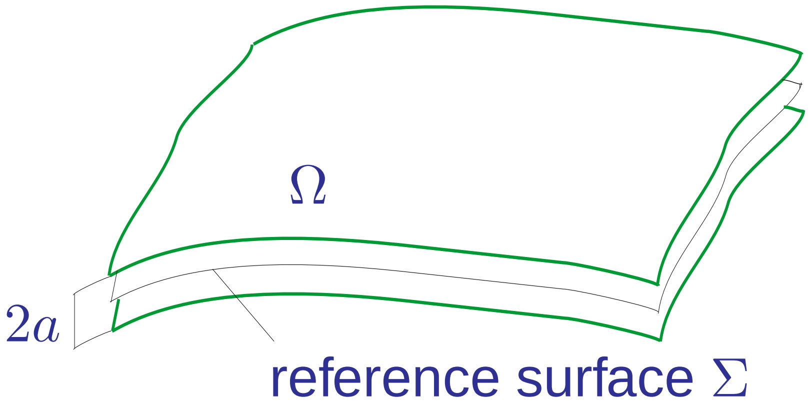

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- If Σ is smooth we can employ the natural curvilinear which now include the intrinsic geometry of Σ
- If the layer is thin the Hamiltonian can be rewritten as

$$H = -g^{-1/2}\partial_\mu g^{1/2} g^{\mu\nu}\partial_\nu - (\partial_u^2)_D + K - M^2 + \mathcal{O}(a)\,;$$

K, M are *Gauss* and *mean curvature* of Σ, respectively

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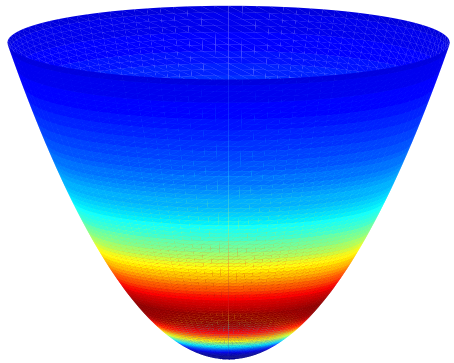
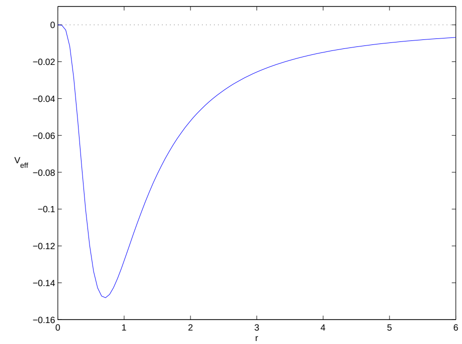
- The leading term $K - M^2$ of the effective potential can be rewritten in terms of principal curvatures of the surface Σ as $-\frac{1}{4}(k_1 - k_2)^2$. It is thus *attractive* unless
  - Σ is *planar*, $k_1 = k_2 = 0$
  - Σ is *spherical*, $k_1 = k_2$, however, an infinite surface Σ clearly *cannot be spherical globally*

Effective Potential $\quad V_{\text{eff}} = -\frac{1}{4}\left(k_{+} - k_{-}\right)^2$

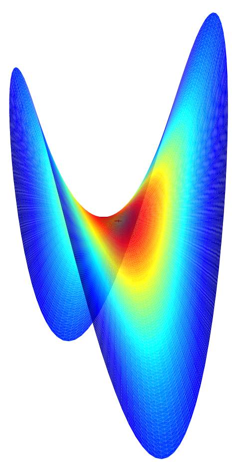
Paraboloid of Revolution $\quad z = x^2 + y^2$

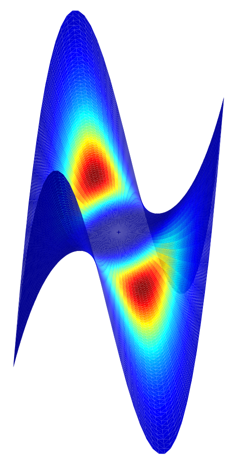




Hyperbolic Paraboloid $\quad z = x^2 - y^2$

Monkey Saddle $\quad z = x^3 - 3xy^2$





The minima of V_{eff} are marked by the dark red colour.

Some layer results

Theorem [Duclos-E-Krejčiřík'01]: Let Σ be smooth, *simply connected* and *asymptotically flat*, then $\sigma_{\rm disc}(-\Delta_D^\Omega) \neq \emptyset$ if

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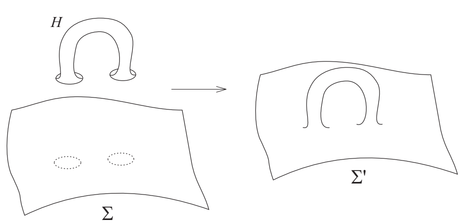
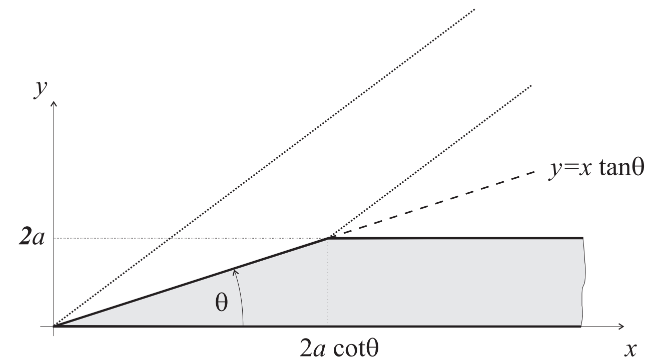
Theorem [Carron-E-Krejčiřík'04]: Let Σ be smooth, asymptotically flat, *not necessarily simply connected*, then

- $\sigma_{\rm disc}(-\Delta_D^\Omega) \neq \emptyset$ holds for genus $g \ge 1$
- If Σ has a *cylindrical end*, there are infinitely many bound states; the same is true if Ω is *locally deformed*



Example: a conical layer

Consider the layer Ω_θ obtained by rotating the figure around the axis $y = x \tan\theta$ for which we have by the above result $\sharp\sigma_{\mathrm{disc}}(-\Delta_D^{\Omega_\theta}) = \infty$



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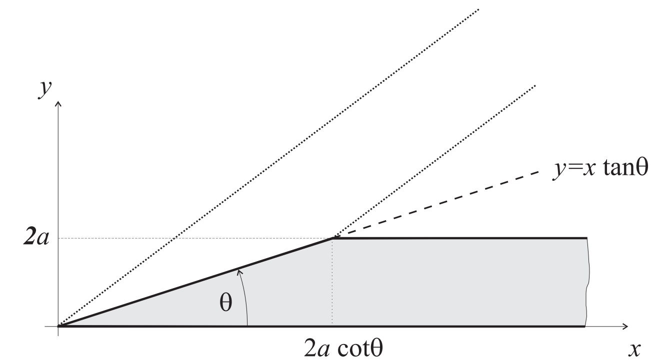
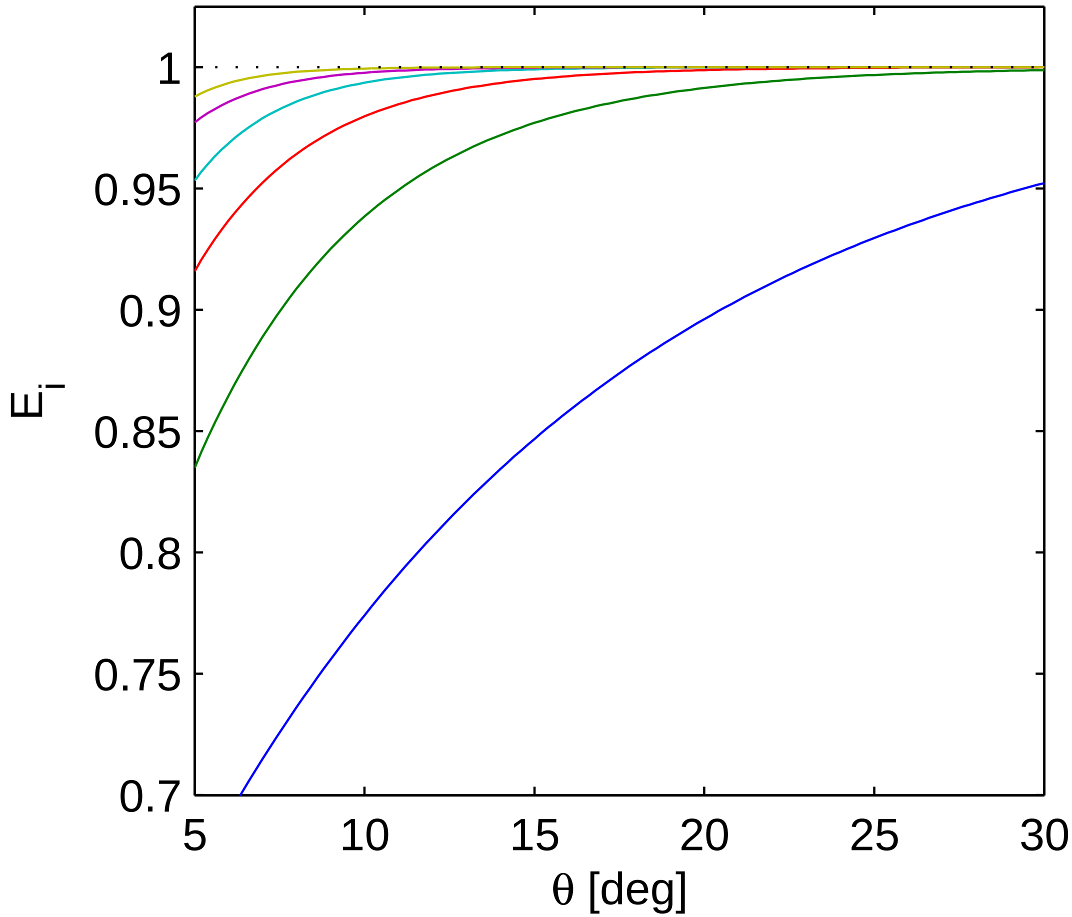


Theorem [E-Tater'10]: For the layer Ω_θ described above

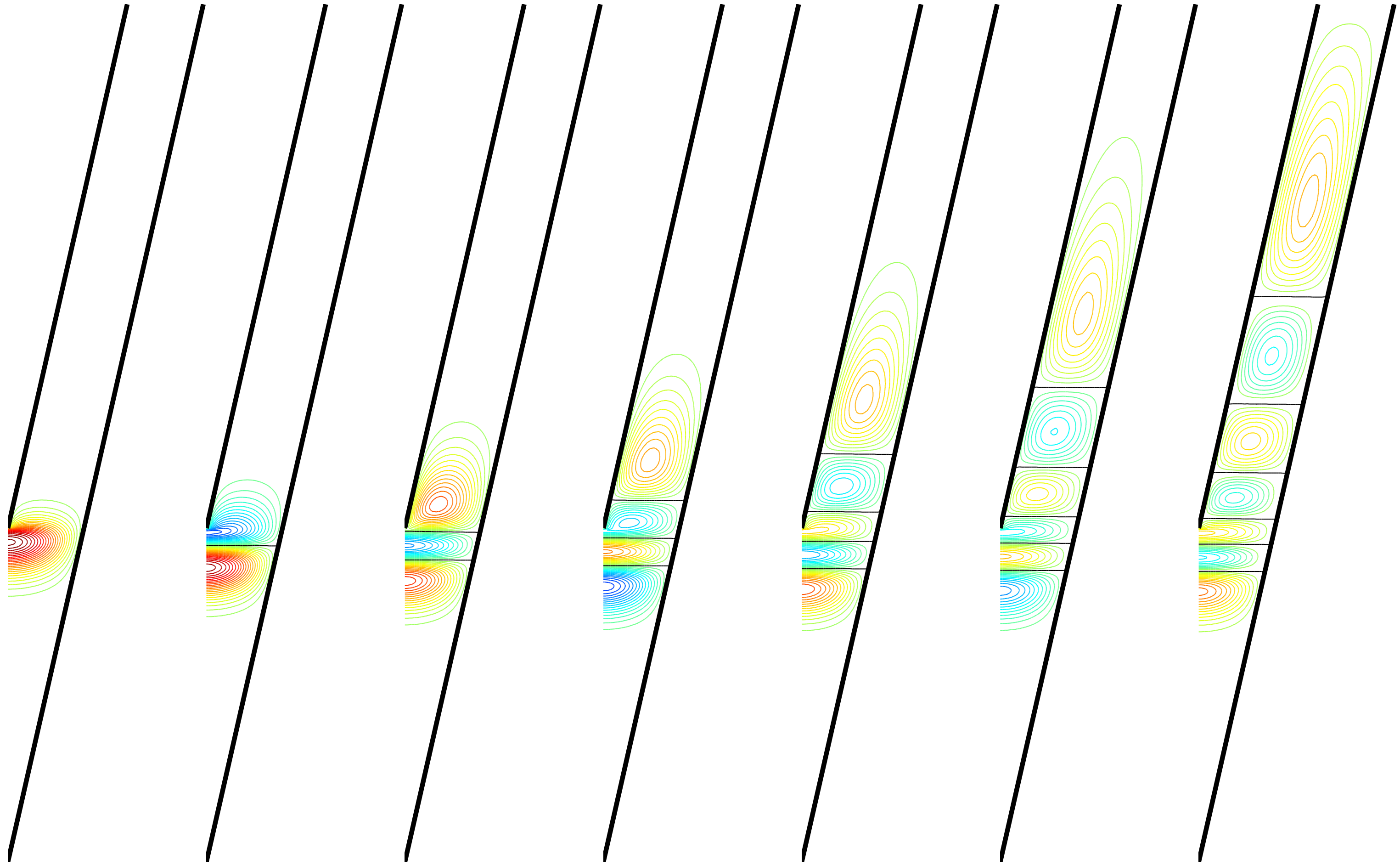
- $\sigma_{\rm disc}(-\Delta_D^{\Omega_\theta})$ contains *s-states only*
- Fix a λ satisfying $\left(\frac{\pi}{d}\right)^2 > \lambda > j_{0,1}^2 d^{-2} \approx 5.783\, d^{-2}$ and a natural number n, then $-\Delta_D^{\Omega_\theta}$ has at least n eigenvalues below λ *for all θ small enough*

Eigenvalues vs. cone opening angle



Plot of the first six eigenvalues

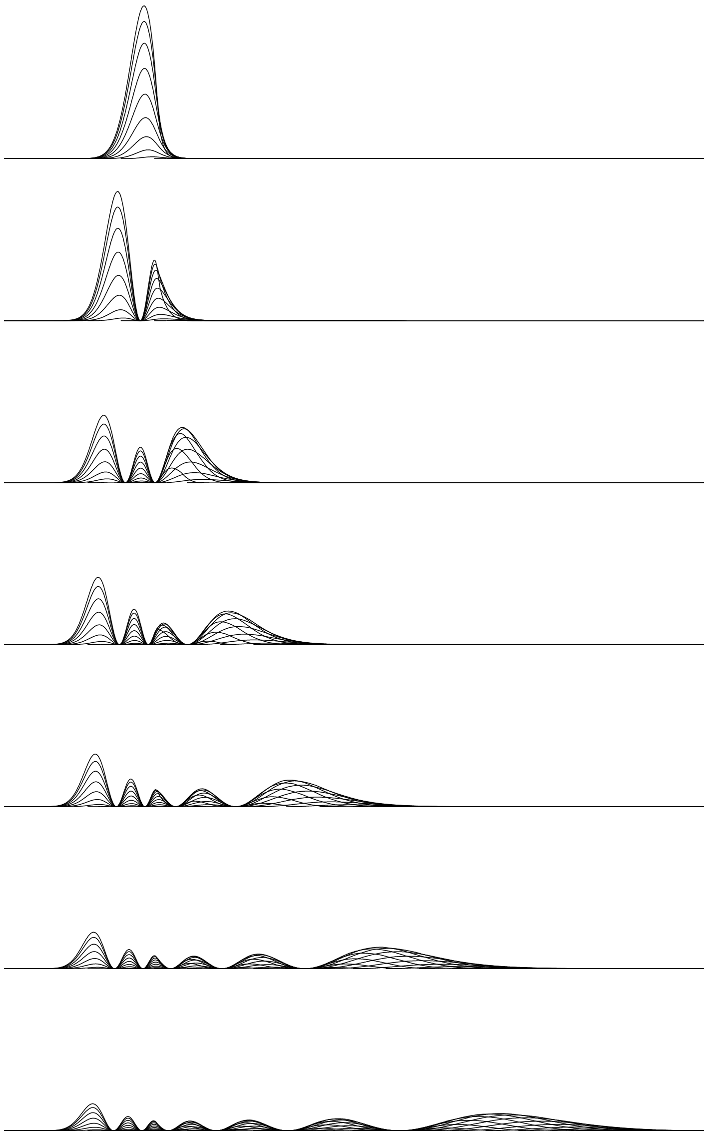
Eigenfunctions for $\theta = 2.5^{\mathrm{o}}$



The contour plot of the first seven eigenfunctions

(five times vertically contracted)

Nodal period doubling



In view of the $-\frac{1}{r^2}$ character of the effective potential the eigenfunctions exhibit a certain kind of self-similar behavior

We illustrate it with the side view of probability density $|\psi|^2$ for the first seven eigenfunctions

Forcing a particle to change dimension

My second topic may seem even more exotic: a quantum motion constrained to a manifold composed of components of generally *different dimensions*, e.g.

- attaching 1D leads to a 2D surface or 3D volume
- coupling 2D surfaces through a point contact, etc.

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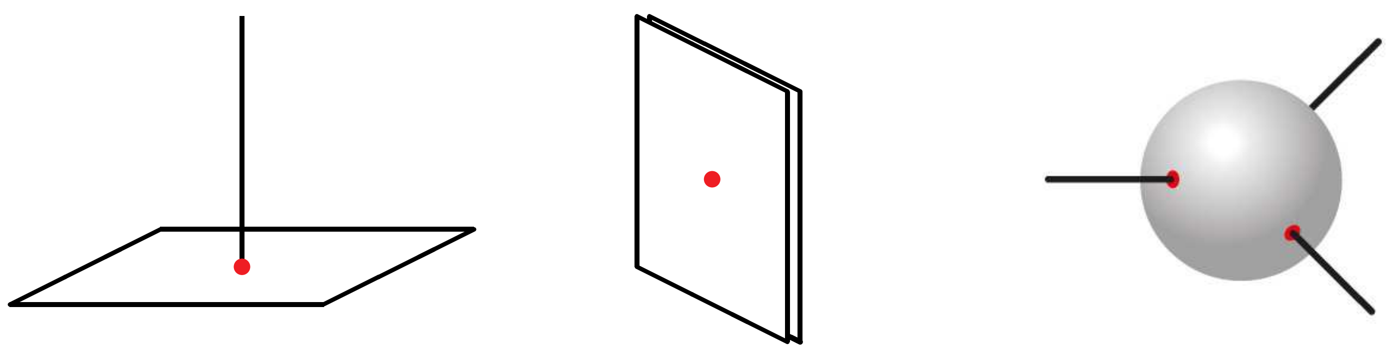

Coupling different dimensions

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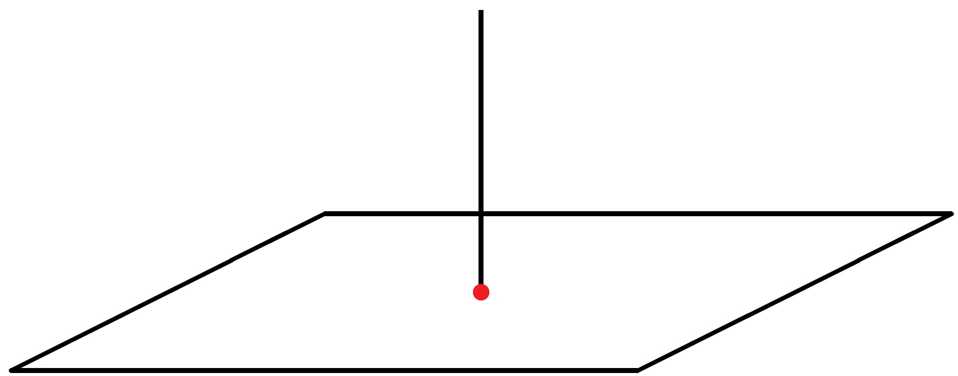
In an archetypal example, $\mathcal{H} = L^2(\mathbb{R}_-) \oplus L^2(\mathbb{R}^2)$, the wave functions are pairs $\phi := \binom{\phi_1}{\Phi_2}$ of square integrable functions



Attaching a lead to a plane

We restrict $\left(-\frac{\mathrm{d}^2}{\mathrm{d}x^2}\right)_{\mathrm{D}} \oplus -\Delta$ to functions vanishing in the vicinity of the junction; the resulting operator is “too small”, in math language it is *symmetric but not self-adjoint*

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Self-adjointness is equivalent to the probability current conservation. Constructing *self-adjoint extensions* is a method going back to J. von Neumann. To characterize them we need *generalized boundary values* at $\vec{x}_0 = 0$

$$\Phi_2(\vec{x}) = L_0(\Phi) \ln |\vec{x}| + L_1(\Phi_2) + \mathcal{O}(|\vec{x}|)$$

(since the plane *two-dimensional*, in the 3D analogue L_0 would be the coefficient at the *pole singularity*)

Admissible couplings

A convenient way to describe s-a couplings is through *boundary conditions*, which can have the following form

$$\begin{aligned} \phi_1'(0-) &= A\phi_1(0-) + B L_0(\Phi_2)\,, \\ L_1(\Phi_2) &= C\phi_1(0-) + D L_0(\Phi_2)\,, \end{aligned}$$

with the coefficients satisfying $A,\, D \in \mathbb{R}$ and $B = 2\pi\bar{C}$

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More generally, one requires $\mathcal{A}\binom{\phi_1}{L_0} + \mathcal{B}\binom{\phi_1'}{L_1} = 0$ where

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It is straightforward to check that any coupling described by these boundary conditions *conserves the probability current*

Transport through point contact

We match the scattering solution $\mathrm{e}^{ikx} + r(k)\mathrm{e}^{-ikx}$ on the lead with the solution $t(k)(\pi kr/2)^{1/2} H_0^{(1)}(kr)$ in the plane using the described boundary conditions.

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with the quantities $\mathcal{D}_\pm(k)$ given by

$$\mathcal{D}_\pm(k) := (A \pm ik)\left[1 + \frac{2i}{\pi}\left(\gamma_{\mathrm{E}} - D + \ln\frac{k}{2}\right)\right] + \frac{2i}{\pi}BC,$$

where $\gamma_{\mathrm{E}} \approx 0.5772$ is Euler's constant

A few remarks

- Notice that the lead is coupled *only to the s-wave part* of the wave function in the plane, the other partial waves are shielded by a *centrifugal barrier*

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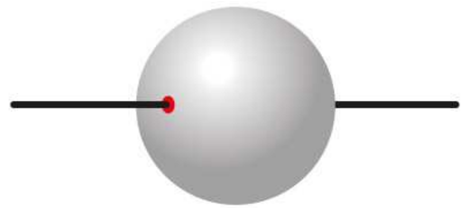
- Notice that *reflection dominates at high energies*, since $|t(k)|^2 = \mathcal{O}((\ln k)^{-2})$ holds as $k \to \infty$

A few remarks

- Notice that the lead is coupled *only to the s-wave part* of the wave function in the plane, the other partial waves are shielded by a *centrifugal barrier*
- Scattering is *nontrivial* if $\mathcal{A} = \begin{pmatrix} A & B \\ C & D \end{pmatrix}$ is not diagonal. For any choice of s-a extension, the on-shell S-matrix is *unitary*, in particular, we have $|r(k)|^2 + |t(k)|^2 = 1$
- Notice that *reflection dominates at high energies*, since $|t(k)|^2 = \mathcal{O}((\ln k)^{-2})$ holds as $k \to \infty$
- a similar analysis can be done also in a more general model where the electron is subject to *spin-orbit coupling* and *mg field*, cf. [E-Šeba'07, Carlone-E'11]

Single-mode geometric scatterers

As an example, consider a sphere with two leads attached



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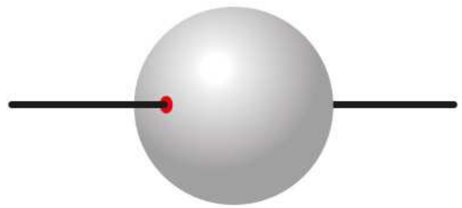
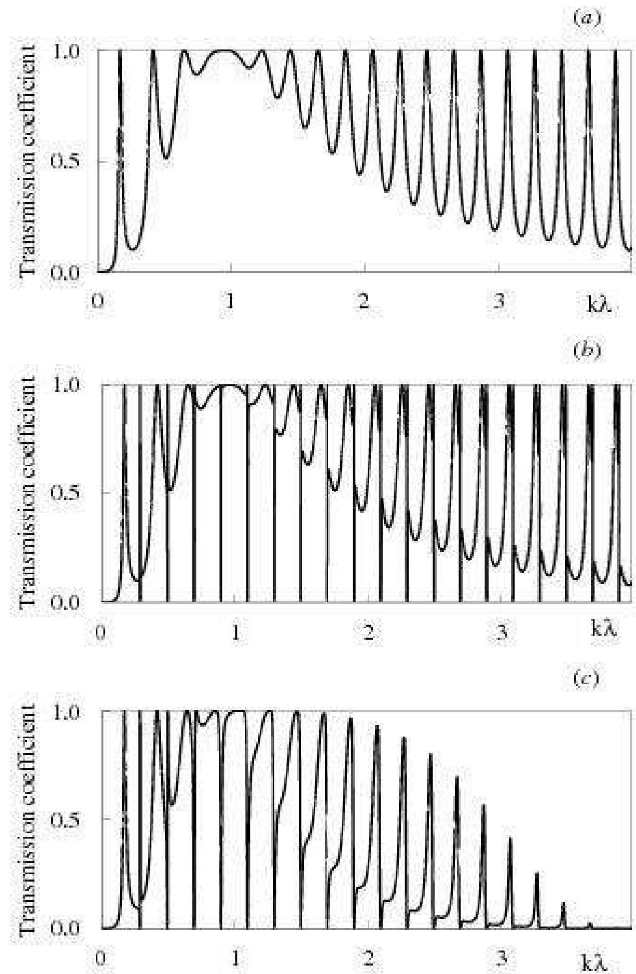


The system was examined in [Kiselev'97; E-Tater-Vaněk'01; Brüning-Geyler-Margulis-Pyataev'02] showing, in particular, the following properties

- scattering *en gross* is not very sensitive to the choice of the coupling, it is *sensitive to relative junction positions*
- there are *numerous resonances* in such systems
- the *background reflection dominates* the picture at high energies, $k \to \infty$

Transmission through the sphere



(a) Junctions at opposed poles, (b) tilt 2^{o}, (c) tilt 4^{o}

(reproduced from [Brüning-Geyler-Margulis-Pyataev'02])

Arrays of geometric scatterers

In a similar way one can analyze scattering on various *"hedgehog" manifolds* composed of compact scatterers, connecting edges and external leads [Brüning-Geyler'03]

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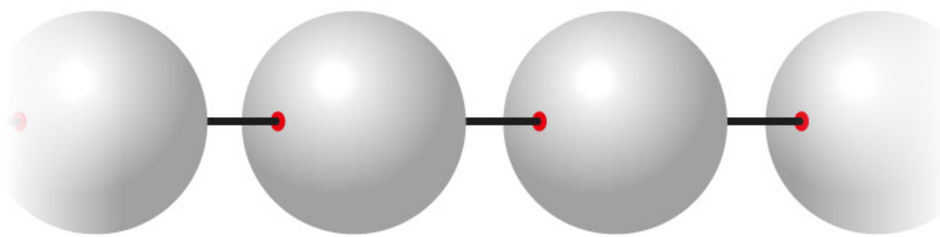
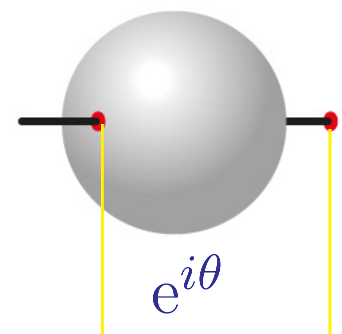
Infinite periodic systems can be treated by the usual trick, *Bloch decomposition* (or “Floquet” for mathematicians)





One has to analyze the discrete spectrum of a single element as a function of the *quasimomentum* θ

How do gaps behave as $k \to \infty$?

Q: Are the scattering properties of such junctions reflected in *gap behavior* of periodic families of geometric scatterers at high energies? And why it should be interesting?

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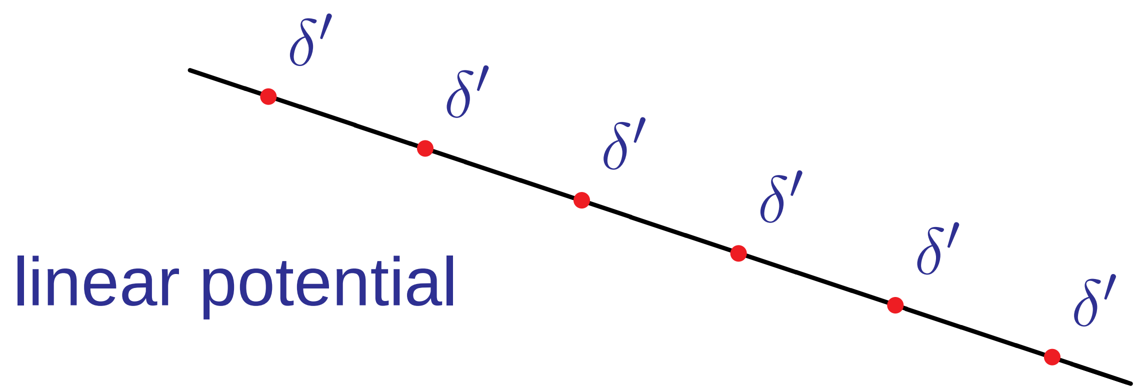
Recall the properties of *singular Wannier-Stark* systems,



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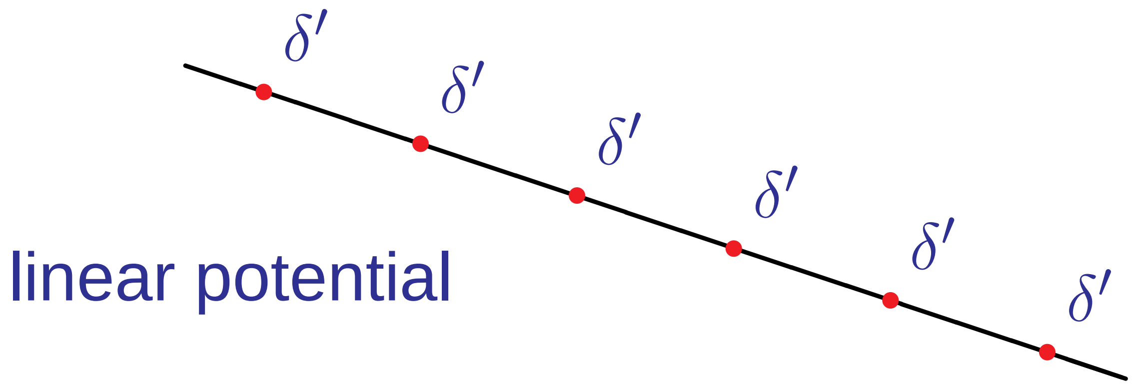

described by the Hamiltonian

$$H = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \alpha \sum_{j\in\mathbb{Z}} (\delta'_{ja}, \cdot)\delta'_{ja} - Fx$$

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- There is *no transport*, $\sigma_{\mathrm{ac}}(H) = \emptyset$ [Avron-E-Last'94]

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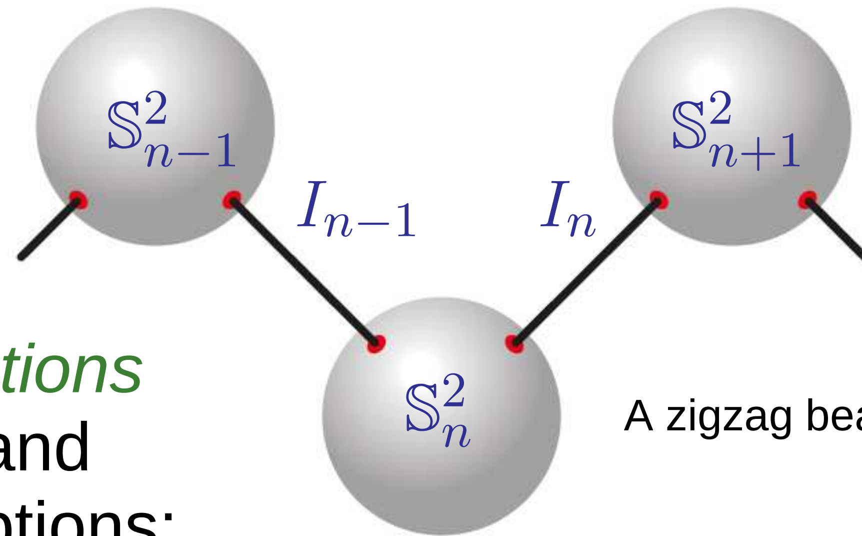
- The δ' interaction has a similar behavior as a sphere scatterer but simpler, *without resonances*. It is conjectured that *coarse-grained* sphere transmission coincides asymptotically with that of δ'

Some periodic systems



A zigzag bead array

Consider *periodic combinations of spheres and segments* and adopt the following assumptions:

- periodicity in one or two directions (one can speak about *“bead arrays”* and *“bead carpets”*)

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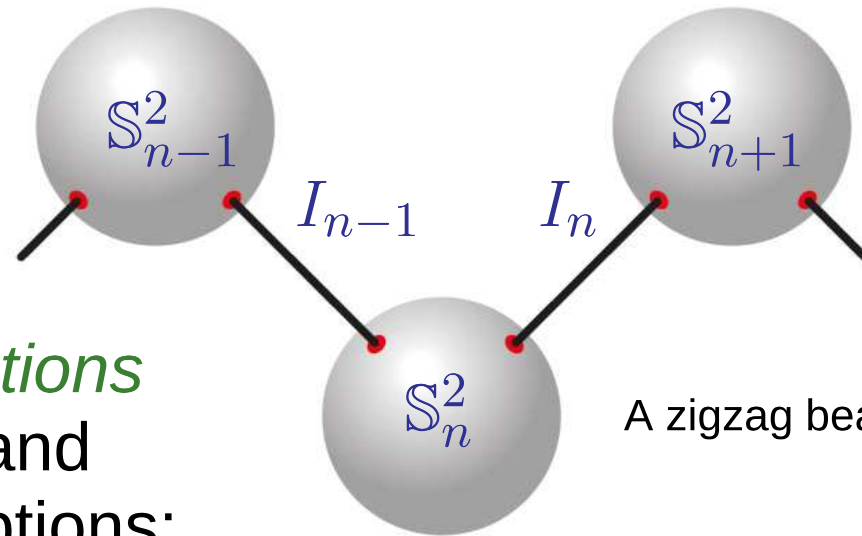

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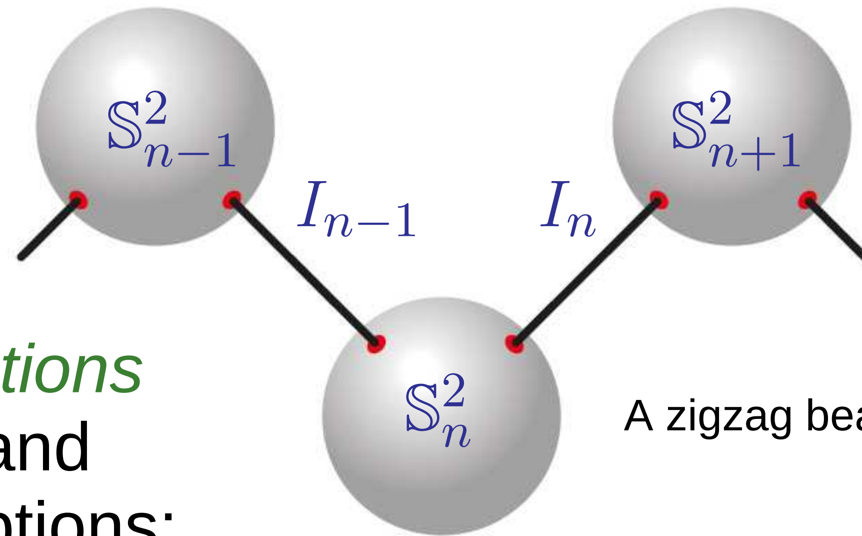

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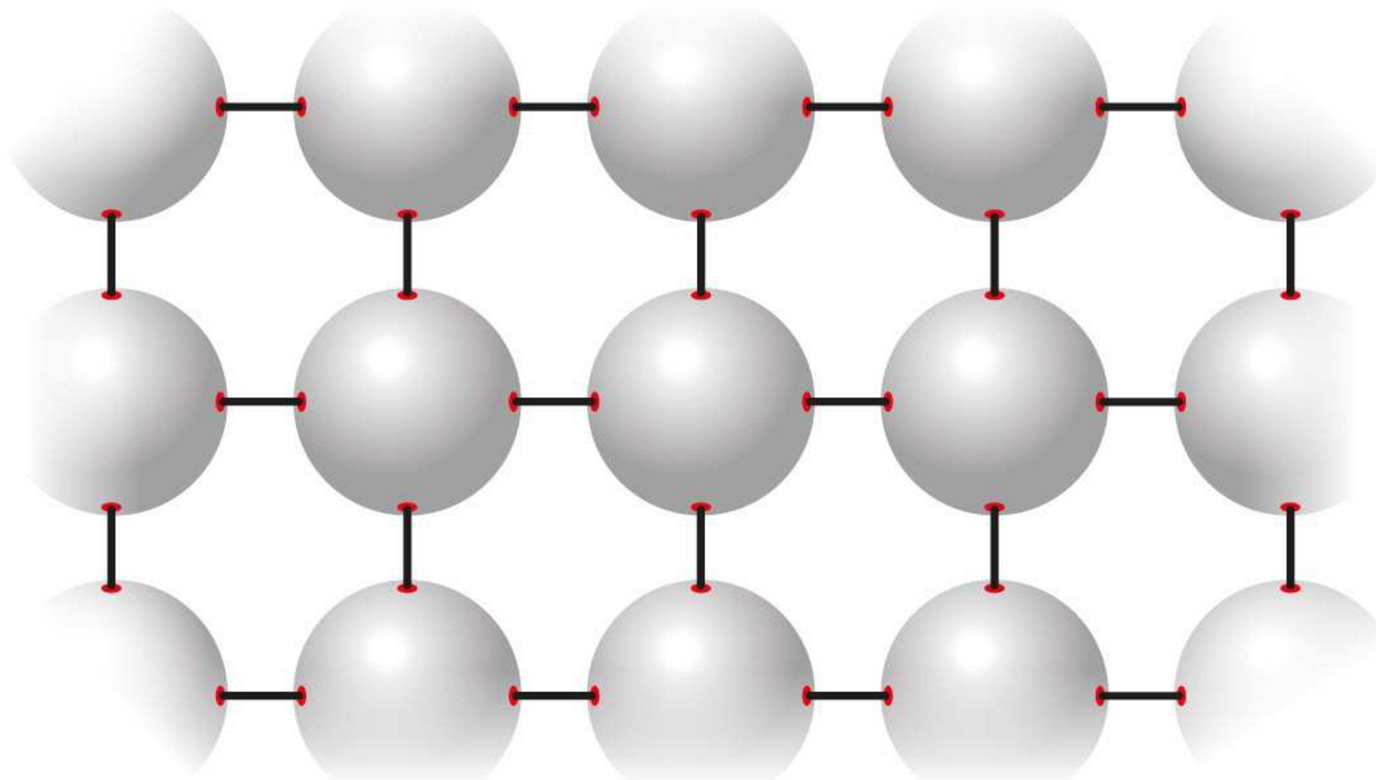
- periodicity in one or two directions (one can speak about *"bead arrays"* and *"bead carpets"*)
- angular distance between contacts equals π or $\pi/2$
- sphere-segment coupling $\mathcal{A} = \begin{pmatrix} 0 & 2\pi\alpha^{-1} \\ \bar{\alpha}^{-1} & 0 \end{pmatrix}$

A bead carpet



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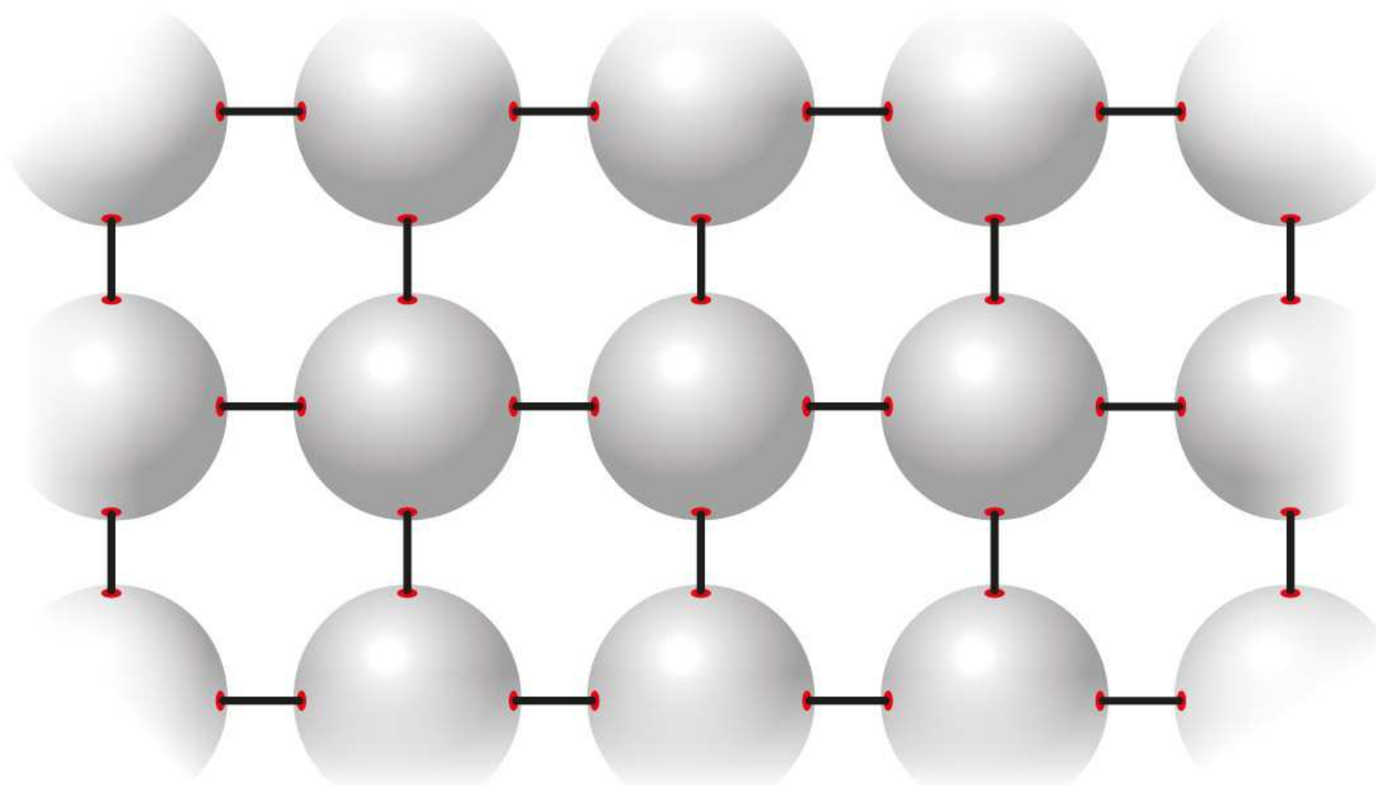
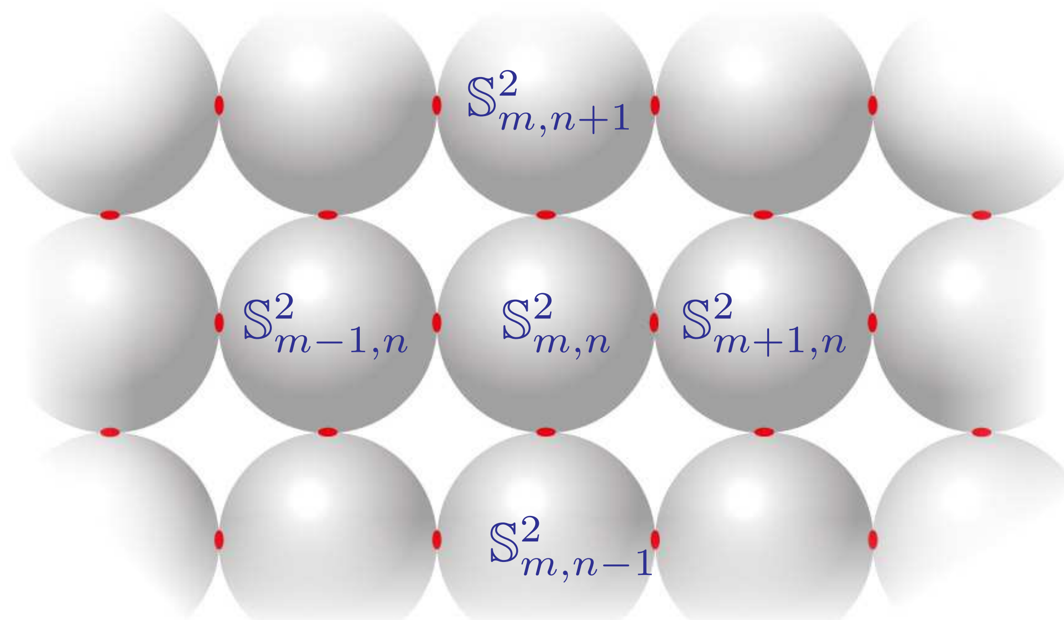


We will call such structures *loose*; we can also consider their *tight* counterparts when the spheres are touching

Tightly coupled spheres



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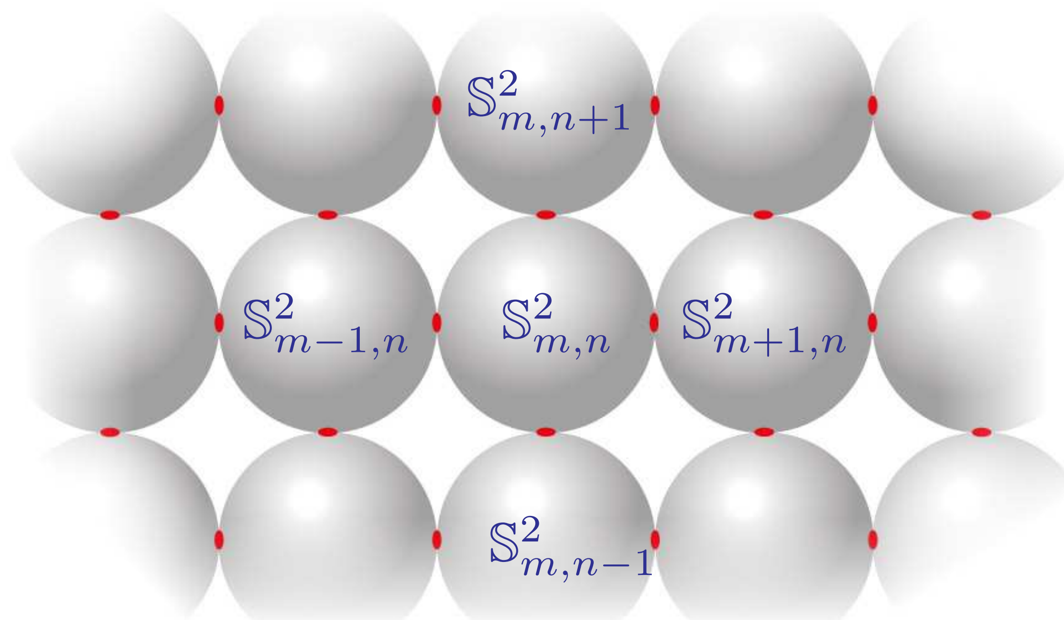

Self-adjoint tightly-coupled systems can be described by the following b.c.

$$L_1(\Phi_1) = AL_0(\Phi_1) + CL_0(\Phi_2)\,,$$
$$L_1(\Phi_2) = \bar{C}L_0(\Phi_1) + DL_0(\Phi_2)$$

with $A, D \in \mathbb{R}$, $C \in \mathbb{C}$. For simplicity we can put $A = D = 0$

Large gaps in periodic manifolds

Denote by $B_n,\, G_n$ the widths of the nth band and gap, respectively; then we have the following claim

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$$\frac{B_n}{G_n} \le c\, n^{-\epsilon}$$

holds as $n\to\infty$ for *loosely connected* systems, where $\epsilon=\frac{1}{2}$ for arrays and $\epsilon=\frac{1}{4}$ for carpets. For *tightly coupled* systems to any $\epsilon\in(0,1)$ there is a $\tilde c>0$ such that the inequality $B_n/G_n \le \tilde c\,(\ln n)^{-\epsilon}$ holds as $n\to\infty$

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Conjecture: The same should hold for other couplings and angular junction distances. The problem is just technical; the dispersion curves are less regular in general

How to choose the coupling?

It depends on detailed knowledge of the junction; the question is about the simplest or “natural” coupling

A possibility is to replace the lead by a *tube of radius* a, disregard effect of the sharp edge at interface, and to compare the *low-energy scattering* in the two cases

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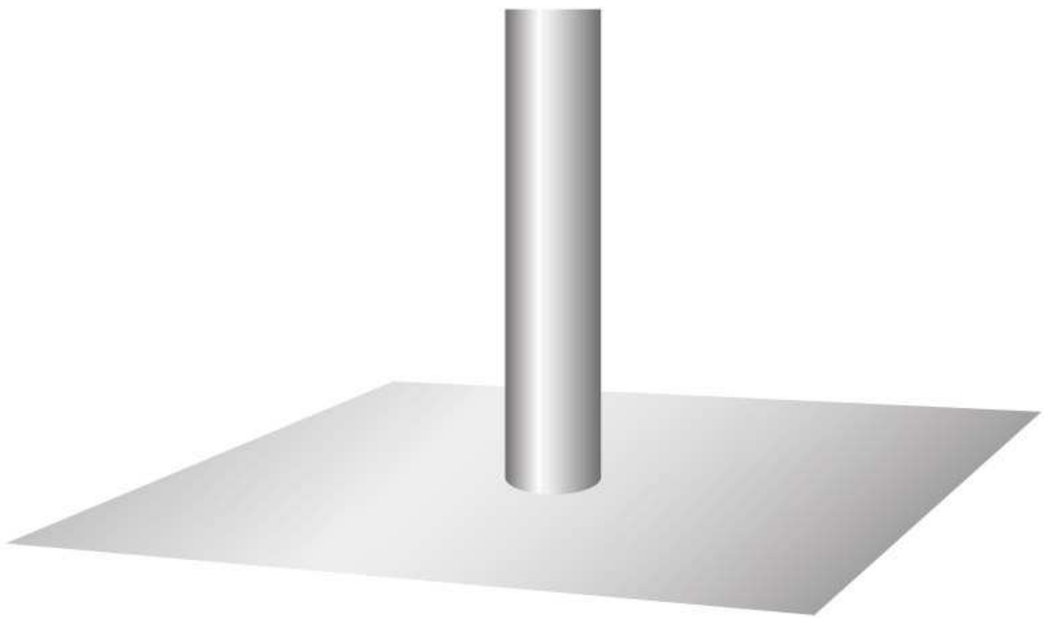

Plane plus tube scattering

Rotational symmetry allows us again to treat each partial wave separately. Given orbital quantum number ℓ one has to match smoothly the corresponding solutions

$$\psi(x) := \begin{cases} e^{ikx} + r_a^{(\ell)}(t)e^{-ikx} & \dots \quad x \le 0 \\ \sqrt{\frac{\pi kr}{2}}\, t_a^{(\ell)}(k) H_\ell^{(1)}(kr) & \dots \quad r \ge a \end{cases}$$

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This yields

$$r_a^{(\ell)}(k) = -\frac{\mathcal{D}_-^a(k)}{\mathcal{D}_+^a(k)}, \quad t_a^{(\ell)}(k) = 4i\sqrt{\frac{2ka}{\pi}}\,\left(\mathcal{D}_+^a(k)\right)^{-1}$$

with

$$\mathcal{D}_\pm^a(k) := (1 \pm 2ika)H_\ell^{(1)}(ka) + 2ka\left(H_\ell^{(1)}\right)'(ka)$$

Choice of coupling parameters

We have

$$|t_a^{(\ell)}(k)|^2 \approx \frac{4\pi}{((\ell-1)!)^2} \left(\frac{ka}{2}\right)^{2\ell-1}$$

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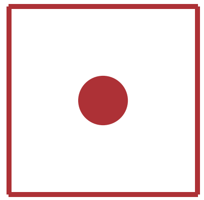
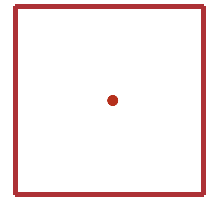
Notice that the “right” s-a extensions depend on a *single parameter*, namely radius of the “thin” component

A digression: Sinai *vs.* Šeba billiard



a prime example of
chaotic classical dynamics



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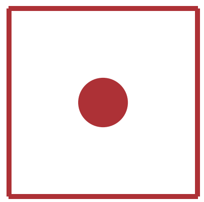

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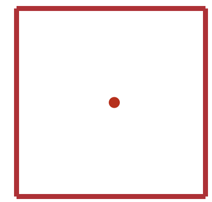

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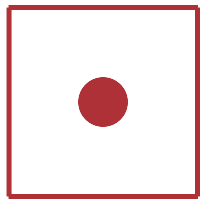

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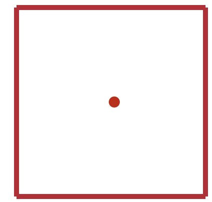

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In particular, the *eigenvalue spacing distribution* is *not* Poissonian as one would expect from a solvable system but exhibits a Wigner-type *level repulsion* characteristic for a *chaotic dynamics*

Resonator with an antenna

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Let a *rectangular resonator* be equipped with an *antenna* which serves a source. Such a system has many resonances; we ask about distribution of their spacings

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Let a *rectangular resonator* be equipped with an *antenna* which serves a source. Such a system has many resonances; we ask about distribution of their spacings

The reflection amplitude for a compact manifold with one lead *naturally* attached at x_0 is easily

$$r(k) = -\frac{\pi Z(k)(1-2ika)-1}{\pi Z(k)(1+2ika)-1},$$

where $Z(k) := \xi(\vec{x}_0;k) - \frac{\ln a}{2\pi}$ with $\xi(\vec{x}_0;k)$ being the *regularized value of Green's function* $G_k(\vec{x}_0,\vec{x})$ as $\vec{x} \to \vec{x}_0$

Comparison with experiment

Match now the model prediction with *experimental results* obtained at *Universität Marburg* using the value $a = 1\,\mathrm{mm}$ and averaging over various $\vec{x}_0$ and $c_1, c_2 = 20 \sim 50\,\mathrm{cm}$

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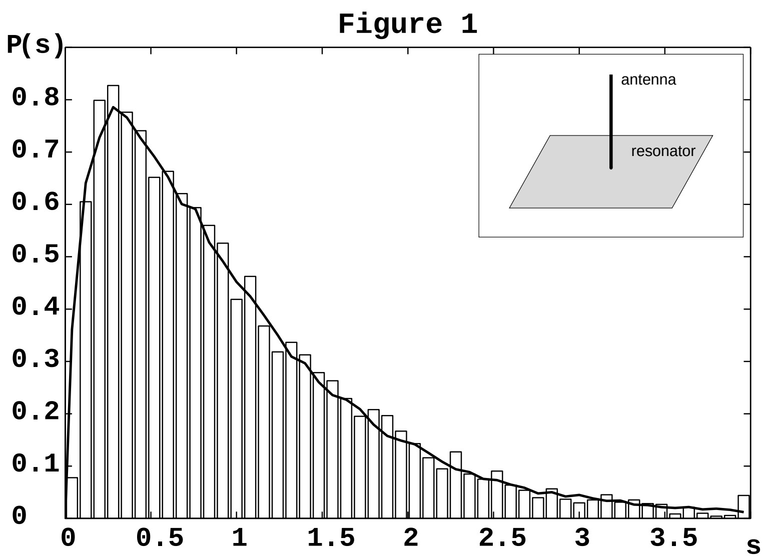

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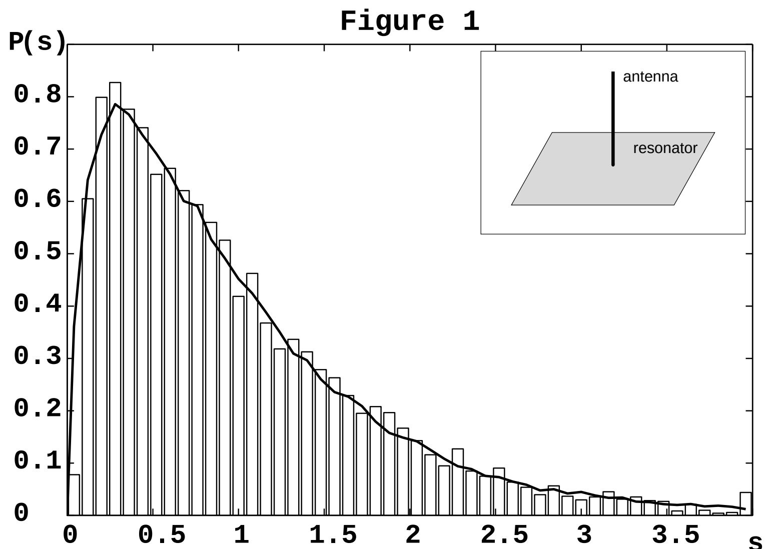

Remark: Agreement was achieved with the *lower third* of measured frequencies – confirming thus validity of our approximation, since shorter wavelengths are comparable with the antenna radius a and $ka \ll 1$ is no longer valid

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- if anything of that inspired you to some thoughts I would be happy to discuss them with you

Thank you for your attention!

Domo arigato!