# Constrained quantum dynamics

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*Doppler Institute*
*for Mathematical Physics and Applied Mathematics*
*Prague*

With thanks to all my collaborators

**A minicourse at the 2nd International Summer School on Advanced Quantum Mechanics**

**Prague, September 2-11, 2021**

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- *Lecture VI:* Spectral effects caused by magnetic fields. Soft quantum waveguides and an outlook.

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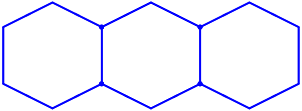

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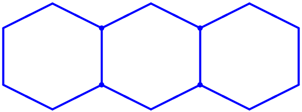

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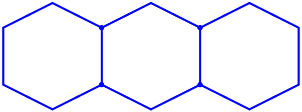

and others – ignoring the double edges marking the bond type – are more than symbols. He conjectured that some electrons form a *graph-shaped frame* in which the remaining ones move.

Using this idea, he managed to calculate spectra of such molecules with $\sim$10% accuracy, a remarkable feat for such a primitive model.

# Matching the wave functions

Doing so, Pauling had to decide how the electron wave functions match at the graph vertices. He choose a simple receipt assuming that they are *continuous* and the *sum of their derivatives vanishes*, that is, what people today mostly call *Kirchhoff conditions*.

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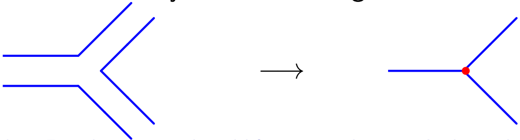

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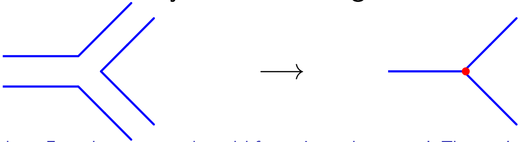

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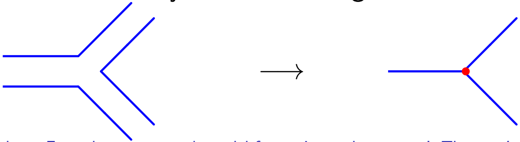

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After that, however, the subject was *happily forgotten* for several decades!

# Rebirth of the concept

The new inspiration came from physics again, namely from the progress in solid state physics. Since the 1980s the fabrication techniques improved allowing us to produce structure so tiny and clean that the electron transport is coherent.

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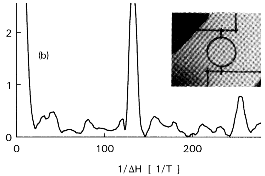


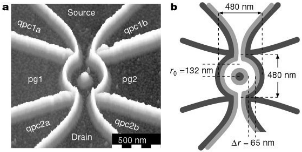


The left figure shows a demonstration of Aharonov-Bohm effect in ring of diameter diameter 784nm made of *gold wire* of width 41nm, the right one a ring-type *heterostructure made of AlGaAs-GaAs*.


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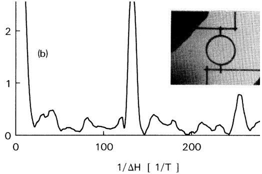


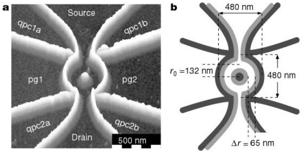


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Quantum graphs appeared be very good models of such systems!

# The sort of graphs we need

Graph theory is venerable part of mathematics which roots can be traced back at least to 1736 when Lenhard Euler answered the question about the *seven bridges of Königsberg*. A graph in this understanding is a collection of *vertices* and of *edges* connecting them in accordance with the graph *adjacency matrix*. The literature on these graphs is immense.

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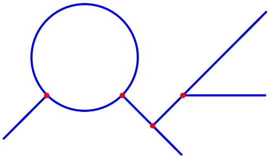

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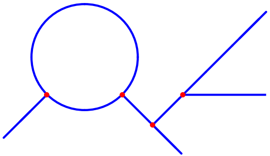

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The two graph concepts are related; we will return to this question later.

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- In addition to Schrödinger, graphs can also support *Dirac operators*. Such models gained importance recently; the reason is that electron motion in *graphene* can be described by *massless Dirac equation*.

W. Bulla, T. Trenkler : The free Dirac operator on compact and noncompact graphs, *J. Math. Phys.* **31** (1990), 1157–1163.

J. Bolte, J.M. Harrison: Spectral statistics for the Dirac operator on graphs, *J. Phys. A: Math. Gen.* **36** (2003), 2747–2769.

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- Graphs are also used to describe other physical processes governed, for example, by the *wave* or *elasticity* equation.


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- The graph literature is extensive indeed; the best source I can recommend to start with is the monograph

  G. Berkolaiko, P. Kuchment: *Introduction to Quantum Graphs*, AMS, Providence, R.I., 2013.

# Vertex coupling

After setting the scene, let us return the concept of quantum graph, in particular to *matching the wave functions*.

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Recall that to define a QM Hamiltonian, in general it is not sufficient to specify its differential symbol. To qualify as an observable, the operator must be *self-adjoint*, $H = H^*$, which for an unbounded operator is a considerably stronger requirement than mere *symmetry*, $H \subset H^*$.

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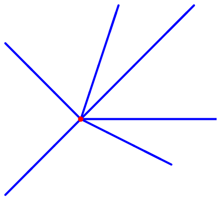
In physicist's language this means to demand that that the *probability current must be preserved*. Let us illustrate that on an example:



The most simple case is a *star graph* with the state Hilbert space $\mathcal{H} = \bigoplus_{j=1}^{n} L^2(\mathbb{R}_+)$ and the particle Hamiltonian acting on $\mathcal{H}$ as $\psi_j \mapsto -\psi_j''$

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These boundary values can be written as columns, $\Psi(0) := \{\psi_j(0)\}$ and $\Psi'(0) := \{\psi'_j(0)\}$, the entries understood as left limits at the endpoint; then the most general self-adjoint matching conditions are of the form

$$A\Psi(0) + B\Psi'(0) = 0,$$

where the $n \times n$ matrices $A, B$ satisfy the conditions

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Naturally, these conditions are non-unique, as $A, B$ can be replaced by $CA, CB$ with a *regular* $C$. This non-uniqueness can be removed by using

$$(U - I)\Psi(0) + i(U + I)\Psi'(0) = 0,$$

where $U$ is a *unitary $n \times n$ matrix*.

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The claim is easy to verify. To see that it is enough to express the squared norms $\|\Psi(0) \pm i\ell\Psi'(0)\|^2_{\mathbb{C}^n}$ and subtract them from each other; the difference is nothing but the *boundary form*,

$$(H\psi, \psi) - (\psi, H\psi) = \sum_{j=1}^{n} (\bar{\psi}_j \psi'_j - \bar{\psi}'_j \psi_j)(0) = 0,$$

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As a consequence, the two vectors having the same norm must be related by an $n \times n$ unitary matrix; this gives $(U - I)\Psi(0) + i\ell(U + I)\Psi'(0) = 0$.

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The claim is easy to verify. To see that it is enough to express the squared norms $\|\Psi(0) \pm i\ell\Psi'(0)\|^2_{\mathbb{C}^n}$ and subtract them from each other; the difference is nothing but the *boundary form*,

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which has to vanish to make the operator self'adjoint.

Note that each term of the sum is, up to the factor $\frac{1}{2}$, nothing but the *probability current* in the $j$th edge, taken in the outward direction.

As a consequence, the two vectors having the same norm must be related by an $n \times n$ unitary matrix; this gives $(U - I)\Psi(0) + i\ell(U + I)\Psi'(0) = 0$.

It seems that we have one more parameter, but it is not important because the matrices corresponding to two different values are related by

$$U' = \frac{(\ell + \ell')U + \ell - \ell'}{(\ell - \ell')U + \ell + \ell'}.$$

Thus we can set $\ell = 1$, which means just a *choice of the length scale*.

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One of them is $H_{\mathrm{D}}$ corresponding to $U = -I$, in other words, each edge component of $H_U$ is a halfline Laplacian with *Dirichlet* boundary condition, $\psi_j(0) = 0$. The spectrum of these operators is easily found, it implies that $\sigma(H_{\mathrm{D}}) = \mathbb{R}_+$ of multiplicity $n$.

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Question: How many of them do we have?

Answer: Their number coincides with the number of eigenvalues of $U$ *in the open upper complex halfplane*. Indeed, the matching condition can diagonalized, and on the appropriate subspaces of $\bigoplus_{j=1}^{n} L^2(\mathbb{R}_+)$ we get $n$ *Robin problems*, $\phi_j'(0) + \tan\frac{\alpha_j}{2}\phi_j(0) = 0$ for the eigenvalue $\mathrm{e}^{i\alpha_j}$ of $U$.

# Examples of vertex coupling

- Denote by $\mathcal{J}$ the $n \times n$ matrix whose all entries are equal to one; then $U = \frac{2}{n+i\alpha}\mathcal{J} - I$ corresponds to the so-called $\delta$ *coupling*,

$$\psi_j(0) = \psi_k(0) =: \psi(0),\; j,k = 1,\dots,n, \quad \sum_{j=1}^{n} \psi_j'(0) = \alpha\psi(0)$$

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- Similarly, $U = I - \frac{2}{n-i\beta}\mathcal{J}$ describes the *$\delta_{\mathrm{s}}'$ coupling*,

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- Another generalization of the 1D $\delta'$ interaction is the *$\delta'$ coupling*:

$$\sum_{j=1}^{n} \psi_j'(0) = 0, \quad \psi_j(0) - \psi_k(0) = \frac{\beta}{n}(\psi_j'(0) - \psi_k'(0)),\; 1 \le j,k \le n$$

with $U = \frac{n-i\alpha}{n+i\alpha} I - \frac{2}{n+i\alpha}\mathcal{J}$ and Neumann edge decoupling for $\beta = \infty$.

# More examples

- The above one-parameter families of vertex couplings exhibit a *permutation symmetry* related to the fact that their $U$'s are combinations of $I$ and $\mathcal{J}$. In general, couplings with this property form a *two-parameter family* described by $U = uI + v\mathcal{J}$ satisfying $|u| = 1$ and $|u + nv| = 1$ corresponding to the conditions

$$(u-1)(\psi_j(0) - \psi_k(0)) + i(u-1)(\psi_j'(0) - \psi_k'(0)) = 0$$

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- Other examples will be mentioned later.

# Quantum waveguides

We return to graphs later, now let us change the topic. Using graphs to model real-world objects like semiconductor *quantum wires* we make certainly some idealizations:

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Let us deal with the first point, forgetting temporarily about the possibility of tuneling; for simplicity supppose that we are in a 2D situation and the particle is confined to a *strip of width* $2a$ in the plane with *hard walls*.

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In the absence of other forces, the Hamiltonian is then the (negative) *Laplacian*, $-\Delta$, and the spectral problem means to solve the equation

$$-\Big(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\Big)\psi(x,y)=\lambda\psi(x,y), \quad x\in\mathbb{R},\ |y|<a,$$

with *Dirichlet boundary condition* describing the hard wall, that is

$$\psi(x,\pm a)=0.$$

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To be specific, consider a curve $\Gamma :\ \mathbb{R} \to \mathbb{R}^2$ assuming that it is *smooth* and *asymptotically straight* and put $\Omega := \{x \in \mathbb{R}^2 : \mathrm{dist}(x, \Gamma) < a\}$; the strip considered above, which denote as $\Omega_0$, refers naturally to the trivial situation when $\Gamma$ is a straight line.

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$$x(s,u) = \big(\Gamma_1(s) - u\dot{\Gamma}_2(s), \Gamma_2(s) + u\dot{\Gamma}_1(s)\big), \quad |u| < a.$$

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We transform $-\Delta$ into these coordinates and remove the Jacobian replacing, with an abuse of notation, $\psi(x)$ with $(1+u\gamma(s))^{1/2}\psi(s,u)$, where $\gamma(s) := (\ddot\Gamma_2\dot\Gamma_1 - \ddot\Gamma_1\dot\Gamma_2)(s)$ is the *signed curvature* of $\Gamma$; then we have to find the spectrum of the following Dirichlet operator in $L^2(\Omega_0)$:

$$H = -\frac{\partial}{\partial s}(1+u\gamma(s))^{-2}\frac{\partial}{\partial s} - \frac{\partial^2}{\partial u^2} + V(s,u),$$

$$V(s,u) := -\frac{\gamma(s)^2}{4(1+u\gamma(s))^2} + \frac{u\ddot\gamma(s)}{2(1+u\gamma(s))^3} - \frac{5}{4}\,\frac{u^2\dot\gamma(s)^2}{(1+u\gamma(s))^4}.$$

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$$H = -\frac{\partial^2}{\partial u^2} - \frac{\partial^2}{\partial s^2} - \frac{1}{4}\gamma(s)^2 + \mathcal{O}(a) \quad \text{as} \;\; a \to 0,$$

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Moral: Listen to your supervisor, but think twice before taking his advice!

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Using the Ansatz $\psi(s,u) = \phi_\lambda(s)\chi_1(u) + \varepsilon f(s,u)$, one can check that choosing appropriately functions $\phi_\lambda(s)$ and $f$ and the number $\varepsilon$, we achieve the goal obtaining the following result:

**Theorem**

*If the strip axis is a $C^4$ smooth curve, not straight but asymptotically straight [leaving out the precise formulation], the the Dirichlet Laplacian in the curved strip has at least one isolated eigenvalue below $\kappa_1^2$.*


J. Goldstone, R.L. Jaffe: Bound states in twisting tubes, *Phys. Rev.* **B45** (1992), 14100–14107.

P. Duclos, P.E.: Curvature–induced bound states in quantum waveguides in two and three dimensions, *Rev. Math. Phys.* **7** (1995), 73–102.

# How it differs from the classical motion?

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However, for a 'quantum bobsleigh' the transverse contribution to the energy is *quantized* so it may not be able to 'jump' from one transverse level to another one.

The comparison is only partly fitting, of course, one can note that a bobsleigh in a rectangular-shaped track would climb nowhere.

# Smoothness is not obligatory

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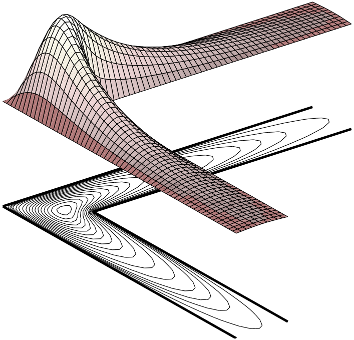
To illustrate this claim, consider $\Omega$ in the shape of an *L-shaped strip*; we choose the width $2a = \pi$ so that $\kappa_1^2 = 1$. Expanding the sought solution to $-\Delta_D^\Omega \psi = \lambda\psi$ into the 'transverse' basis, one can prove that the operator has a single eigenvalue $\approx 0.929$; the corresponding eigenfunction is



P.E., P. Šeba, P. Šťovíček: On existence of a bound state in an L-shaped waveguide, *Czech. J. Phys.* **B39** (1989), 1181–1191.

# Other geometries

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The *essential* (absolutely continuous) *spectrum* of the Hamiltonian $H$ starts now at $\left(\frac{\pi}{d}\right)^2$, where $d = \max\{d_1, d_2\}$ and we have

**Theorem**

*The discrete spectrum of H is nonempty for any $a > 0$ and*

$$\sharp\sigma_{\mathrm{disc}}(H) \geq \frac{2a}{d}\sqrt{1 - \left(\frac{d}{d_1 + d_2}\right)^2}$$

P.E., P. Šeba, M. Tater, D. Vaněk: Bound states and scattering in quantum waveguides coupled laterally through a boundary window, *J. Math. Phys.* **37** (1996), 4867–4887.

# Example: two particular cases

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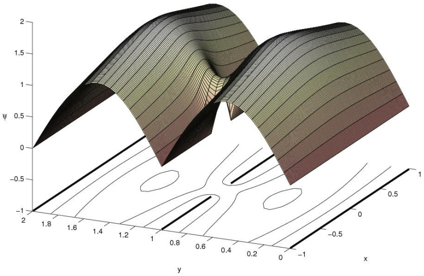


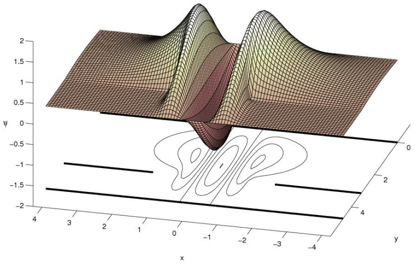

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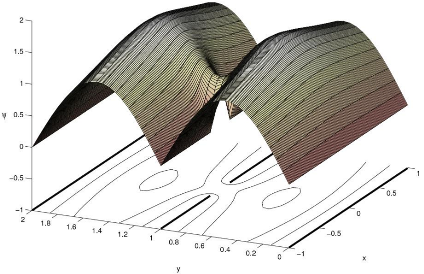


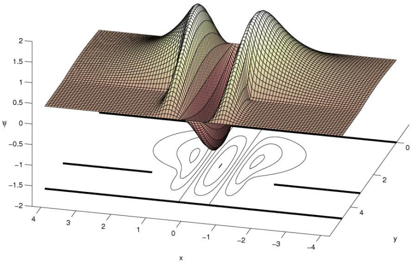


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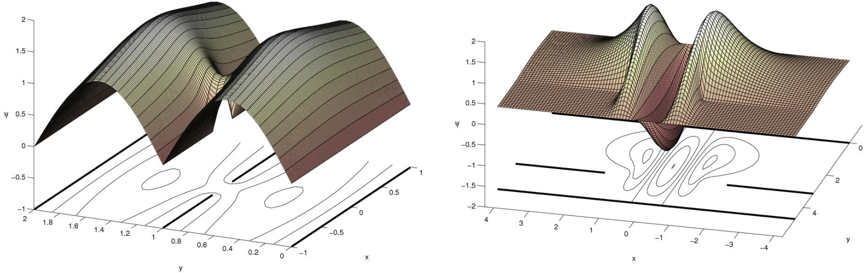


In particular, this example illustrates well the *purely quantum nature* of the effect: a classical particle in such a system *cannot be trapped* except for the (*phase-space measure zero!*) events of reflections, either from the window edges or perpendicular to the walls.

# A detour: Šeba billiard

Of course, this is not the only example illustrating *profound differences* between the classical and quantum mechanics. Let us mention one more, remotely related, which concerns a *chaotic behavior*.

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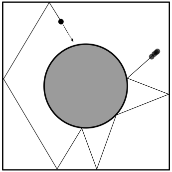

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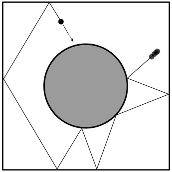

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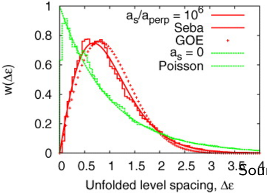


Source: [SAYO'10]


P. Šeba: Wave chaos in singular quantum billiard, *Phys. Rev. Lett.* **64** (1990), 1855–1858.

C. Stone, Y.A. El Aoudi, V.A. Yurovsky, M. Olshanii1: Two simple systems with cold atoms: quantum chaos tests and non-equilibrium dynamics, *New J. Phys.* **12** (2010), 055022.

# More results about waveguides

- The results can be tested experimentally in *flat electromagnetic waveguides*.

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- Similar results hold for three-dimensional bent tubes of *circular cross section*.
- If the cross section *is not circular*, we have to consider the *twisting* which, in contrast to the bending, produces a *repulsive* interaction.

For many more results see

P.E., H. Kovařík: *Quantum Waveguides*; *xxii* + 382 p.; Springer International, Heidelberg 2015.

# Quantum layers

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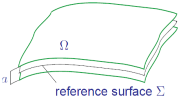


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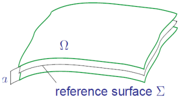


We consider a particle confined to a *hard-wall layer* of width $2a$ built over an *infinite, smooth, non-planar, asymptotically flat* surface $\Sigma$. As in the previous case we can use the curvilinear coordinates in which, for *thin layers*, we have

$$H = -\frac{\partial^2}{\partial u^2} - g^{-1/2}\frac{\partial}{\partial s_\mu} g^{1/2} g^{\mu\nu} \frac{\partial}{\partial s_\nu} + K - M^2 + \mathcal{O}(a),$$

where $g$ is *metric tensor* of the surface $\Sigma$, and $K$, $M$ are its *Gauss* and *mean* curvatures, respectively

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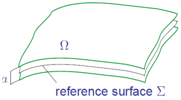


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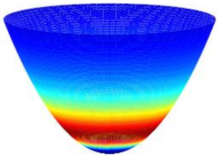
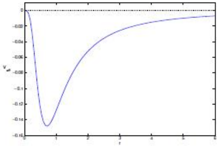
where $g$ is *metric tensor* of the surface $\Sigma$, and $K$, $M$ are its *Gauss* and *mean* curvatures, respectively. Since $K = k_1 k_2$ and $M = \frac{1}{2}(k_1 + k_2)$, the leading term of the effective potential, $K - M^2 = -\frac{1}{4}(k_1 - k_2)^2$, is again of the *attractive* nature, vanishing only on *planes* and *spheres*.

# The effective potential in a thin layer

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

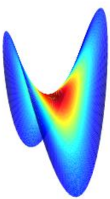
Paraboloid of Revolution $z = x^2 + y^2$

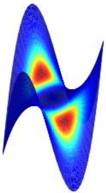




Hyperbolic Paraboloid $z = x^2 - y^2$

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





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

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**Theorem**

*If the surface $\Sigma$ is $C^4$ smooth non-planar and $\mathcal{K} = \int_\Sigma K \, \mathrm{d}\Sigma \le 0$ we have $\inf \sigma(H) < \kappa_1^2$. If $\Sigma$ is asymptotically flat [leaving out again the precise formulation], the the Dirichlet Laplacian has at least one isolated eigenvalue below $\kappa_1^2$.*

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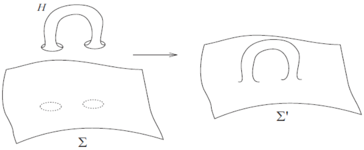
Furthermore, the *Cohn-Vossen inequality* states that

$$\mathcal{K} \le 2\pi\,(2 - 2h - e),$$

where $h$ is the *genus* of $\Sigma$ and $e$ is the *number of ends*



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Hence $\mathcal{K} < 0$ whenever $h \geq 1$ and we have

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*Conclusions of the previous theorem hold whenever $\Sigma$ is not conformally equivalent to the plane.*


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But layers of positive Gauss curvature reveal other interesting property, namely that the spectral properties may depend on the *global geometry* of the region to which the particle is confined.

# Example: conical layers

Consider a hard-wall layer of the thickness $\pi$ built over *conical surface* of an opening angle $\pi - 2\theta$ for some $\theta \in (0, \frac{1}{2}\pi)$,

$$\Sigma_\theta := \{(r, \phi, z) \in \mathbb{R}^3 :\; z = r\,\sin\theta,\; \phi \in [0, 2\pi)\}$$

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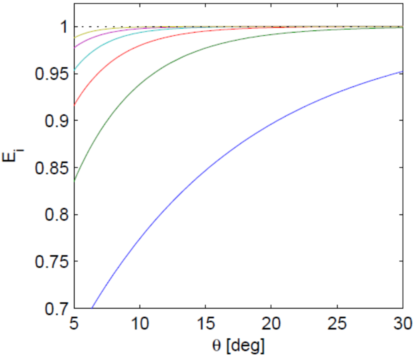
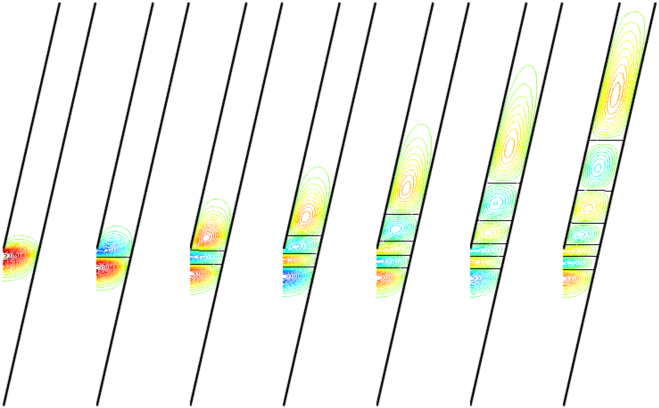
The discrete spectrum infiniteness is related to the fact that the *geodetic circles* on $\Sigma_\theta$ are *shorter* than their counterparts in the plane, which means that the effective attractive potential that behaves asymptotically as $\frac{c}{r^2}$.

# Conical layer eigenvalues



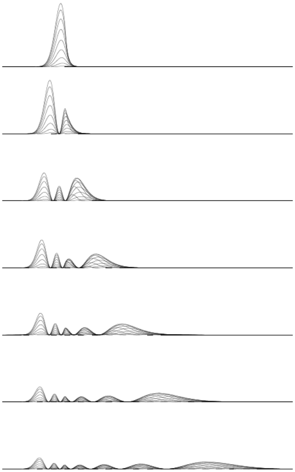

Plot of the dependence of the first six eigenvalues on $\theta$

# Conical layer eigenfunctions



Plot of the first seven eigenvalues for $\theta = \frac{5\pi}{36}$

# Conical layer probability distributions



Plot of the radial cuts of the first seven probability distributions for $\theta = \frac{5\pi}{36}$

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- Quantum waveguides, layers, and other structures of this type offer a demonstration that geometric constraints can induce *nontrivial spectral and dynamical properties*.
- They also show that such system may exhibit behavior of *purely quantum nature* which defies our intuition rooted in our everyday ‘classical’ experience.