Constrained quantum dynamics

Pavel Exner

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

Ubi materia, ibi geometria

Even if Kepler wrote this in a particular context and physics of his cosmography was wrong, the phrase appeared to have a deeper meaning.

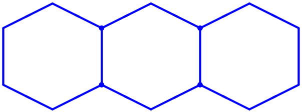
With this motto in mind, here is the *outline of the course:*

- *Lecture I:* Quantum graphs and waveguides, where they come from and what they are good for.
- *Lecture II:* How to match the wavefunctions at the branching points and it does mean physically.
- *Lecture III:* Transport in quantum graphs: resonances, spectral bands, and the Bethe-Sommerfeld property.
- *Lecture IV:* Graphs violating the time-reversal invariance. Taking tunneling into account: the leaky graph model.
- *Lecture V:* Asymptotical properties of leaky graph spectra. Spectral optimization problems for graphs and waveguides.
- *Lecture VI:* Spectral effects caused by magnetic fields. Soft quantum waveguides and an outlook.

Pauling's insight

Constrained motions can be found in many parts of physics, often a distinction between *natural* and *artificial* constraints being not sharp.

In QM an example of a constrained motion appeared in its early days when *Linus Pauling* suggested that the pictures describing molecules of *aromatic hydrocarbons*, like benzene, napfthalene, anthracene sketched here



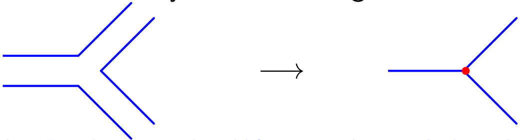
and others – ignoring the double edges marking the bond type – are more than symbols. He conjectured that some electrons form a *graph-shaped frame* in which the remaining ones move.

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*.

This choice requires a justification as it is *not the only possibility*. The answer was proposed seventeen years later using another natural idea:



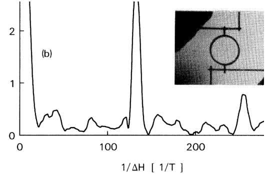
K. Ruedenberg, C.W. Scherr: Free–electron network model for conjugated systems, I. Theory, *J. Chem. Phys.* **21** (1953), 1565–1581.

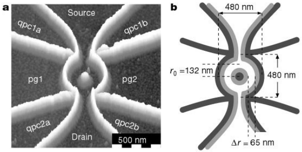
By a *formal use* of Green's formula, they showed that the *squeezing limit* of free motion in a branched tube with *Neumann boundary* yields nothing but the Kirchhoff conditions used by Pauling.

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.





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*.

R.A. Webb, S. Washburn, C.P. Umbach, R.B. Laibowitz: Observation of h/e Aharonov-Bohm oOscillations in normal-metal rings, *Phys. Rev. Lett.* **54** (1985), 2696–2699.

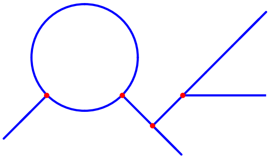
A. Fuhrer, S. Lüscher, T. Ihn, T. Heinzel, K. Ensslin, W. Wegscheider, M. Bichler: Energy spectra of quantum rings, *Nature* **413** (2001), 822–825.

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.

We need more, however, our graphs have to *metric* ones, meaning that we assign a *length* with each edge and can identify it with a *line segment*. This allows us to consider *differential operators* on them associated with QM observables:



Hamiltonian: $-\frac{\mathrm{d}^2}{\mathrm{d}x_j^2} + v(x_j)$
on graph edges,
boundary conditions at vertices

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

Remarks

- Unless stated otherwise, we use units in which $\hbar = 2m = 1$, etc.
- There are numerous materials of which such graph-like systems are constructed. We mentioned *semiconductors* or *metals* materials, one can also use *carbon nanotubes*, etc.
- Observed from the stationary point of view, it is not surprising that properties of such systems can be successfully simulated by *microwave networks* built of optical cables.

O. Hul, S. Bauch, P. Pakoński, N. Savytskyy, K. Życzkowski, L. Sirko: Experimental simulation of quantum graphs by microwave networks, *Phys. Rev.* **E69** (2004), 056205.

- Particles confined to a graph can be under influence of *external fields*. Here we mostly assume that, apart of the constraint, the motion is free, however, we will also pay attention to *magnetic effects*.
- 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.

Remarks

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

P. Freitas, J. Lipovský: Eigenvalue asymptotics for the damped wave equation on metric graphs, *J. Diff. Eqs* **263** (2013), 2780–2811.

J.-C. Kiik, P. Kurasov, M. Usman: On vertex conditions for elastic systems, *Phys. Lett.* **A379** (2015), 1871–1876.

- One can also consider other than linear dynamics on graphs, for instance, the *nonlinear Schrödinger equation* used as effective description of many particle systems, and others.

D. Noja: Nonlinear Schrödinger equation on graphs: recent results and open problems, *Phil. Trans. Roy. Soc.* **A372** (2014), 20130002.

M. Cavalcante: The Korteweg-de Vries equation on a metric star graph, *ZAMP* **69** (2018), 124.

- Graphs proved to be a versatile tool to study *quantum chaos*.

T. Kottos, U. Smilansky: Quantum chaos on graphs, *Phys. Rev. Lett.* **79** (1997), 4794–4797.

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

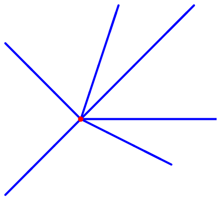
G. Berkolaiko, P. Kuchment: *Introduction to Quantum Graphs*, AMS, Providence, R.I., 2013.

Vertex coupling

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

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*, $H \subset H^*$.

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 $\psi_j \mapsto -\psi_j''$

Vertex coupling

Since the operator is of second order, the boundary condition involve the values of functions and the first *outward* derivatives at the vertex.

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

- $\mathrm{rank}\,(A, B) = n$
- AB^* is *Hermitean*

V. Kostrykin, R. Schrader: Kirhhoff's rule for quantum wires, *J. Phys. A: Math. Gen.* **32** (1999), 595–630.

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*.

Vertex coupling

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*,

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

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 jth 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*.

Why we should care about different couplings?

The answer to this question is: from the simple reason – because they describe a *different physics*. We will encounter various manifestation of this fact but let us illustrate the claim on the example of star graph of n edges, denoting its different Hamiltonians as H_U.

One of them is H_{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.

For any U we have $\sigma_{\mathrm{ess}}(H_U) = \mathbb{R}_+$, because $(H_U - z)^{-1} - (H_{\mathrm{D}} - z)^{-1}$ is an operator of *finite rank* (equal to n) but in addition, there may be *negative eigenvalues*.

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 *δ coupling*,
$$\psi_j(0) = \psi_k(0) =: \psi(0),\ j,k = 1,\dots,n, \quad \sum_{j=1}^{n} \psi_j'(0) = \alpha\psi(0)$$
with 'coupling strength' $\alpha \in \mathbb{R}$; $\alpha = \infty$ gives the Dirichlet $U = -I$
- On the other hand, $\alpha = 0$ is the *Kirchhoff condition* representing a 'free motion'. The name is unfortunate – 'free' or 'standard' would be better – but it stuck.
- Similarly, $U = I - \frac{2}{n-i\beta}\mathcal{J}$ describes the *$\delta_{\rm s}'$ coupling*,
$$\psi_j'(0) = \psi_k'(0) =: \psi'(0),\ j,k = 1,\dots,n, \quad \sum_{j=1}^{n} \psi_j(0) = \beta\psi'(0)$$
with $\beta \in \mathbb{R}$. For $\beta = \infty$ we get the *Neumann* decoupling; the case $\beta = 0$ is sometimes referred to as *anti-Kirchhoff condition*.
- Another generalization of the 1D δ' interaction is the *δ' 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

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

$$(u-1+nv)\sum_{k=1}^{n}\psi_k(0) + i(u-1+nv)\sum_{k=1}^{n}\psi_k'(0) = 0$$

- This is still a small subset among all couplings which depend on n^2 *real parameters*. Symmetries allow us to distinguish other subfamilies. For instance, since the time reversal is (in spinless systems) realized through complex conjugation, H_U describes a *time-reversal-invariant* dynamics iff the matrix U is invariant w.r.t. transposition, $U = U^{\mathrm{t}}$.
- 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:

- real wires have a *nonzero diameter*
- the confinement is not perfect, in particular, quantum *tuneling* is possible between different wires (or different part of the same wire)

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*.

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

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

A 2D quantum waveguide

This is easy to solve by *separation of variables*: the transverse problem, $-\chi''(y) = \kappa^2\chi(y)$, has a discrete spectrum,

$$\kappa_n^2 = \left(\frac{\pi n}{2a}\right)^2,\ \chi_{2n-1}(y) = \frac{1}{\sqrt{a}}\cos\kappa_{2n-1}y,\ \chi_{2n}(y) = \frac{1}{\sqrt{a}}\sin\kappa_{2n}y,\ n = 1, 2, \dots,$$

while the spectrum of the longitudinal part is $[0, \infty)$. Consequently, the spectrum of the full problem in $[\kappa_1^2, \infty)$ with the *generalized eigenfunctions*

$$\chi_n(y)\,\mathrm{e}^{\pm ikx} \quad \text{referring to energy} \quad \kappa_n^2 + k^2$$

It is so simple that you may wonder why I am mentioning it at all. The reason will become with obvious when we note a *nontrivial geometry* may change the picture. As the simplest example suppose that the *strip is bent*.

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 Ω_0, refers naturally to the trivial situation when Γ is a straight line.

A bent Dirichlet strip

Classical intuition suggests that *nothing much happens*: the particle may reflect from the walls but *the only closed trajectories* are those perpendicular to the strip axis, a zero measure set in the phase space.

To see what happens with a quantum particle, we have to solve the spectral problem, $-\Delta_{\mathrm{D}}^{\Omega}\psi = \lambda\psi$, for the corresponding Dirichlet Laplacian. A useful trick is to parametrize Ω using locally orthogonal *curvilinear coordinates* s, u, parallel and perpendicular to the strip axis, respectively,

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

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 Γ; then we have to find the spectrum of the following Dirichlet operator in $L^2(\Omega_0)$:

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

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

A bent Dirichlet strip

In this way, we have to solve an equation on a straight strip but a more complicated; the geometry was now *translated into the coefficients*.

It is not as bad as it looks at a glance. First of all, since Ω is supposed to be *asymptotically straight*, it is not difficult to check that the bend keeps the essential spectrum preserved, $\sigma(-\Delta_{\mathrm{D}}^{\Omega}) = [\kappa_1^2, \infty)$. Moreover, we have

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

and as a 1D Schrödinger operator with a *purely attractive potential*, the longitudinal part has *at least one negative eigenvalues* whenever $\gamma \neq 0$.

Remark: Limits like $a \to 0$ were studied in the 1970s as a tool for *quantization on manifolds*. In particular, Jiří Tolar computed them in all dimensions and codimensions – but his supervisor told him it was good for nothing so he put it into his drawer and published it only many years later:

J. Tolar: On a quantum mechanical d'Alembert principle, in *Group Theoretical Methods in Physics*, Lecture Notes in Physics, vol. 313, Springer, Berlin 1988; pp. 268-274.

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

A bent Dirichlet strip

But we can do better, without restriction on the strip width. Consider any $a > 0$ for which the strip boundary is still smooth, $a\|\gamma\|_\infty < 1$, and the strip *does not intersect itself*.

We apply the *variational method:* if we find a function $\phi \in D(H)$ such that $(\psi, H\psi) < \kappa_1^2\|\psi\|^2$, the spectrum threshold would be *below* κ_1^2.

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 ε, 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 κ_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?

Trying to understand where this effect might come from we may think of what classical mechanics tells us about a *bobsleigh* moving down through a twisting, banked, iced track. As we all know in the curved part the conservation laws make the bobsleigh 'climb' the track wall,

Source: Wikipedia

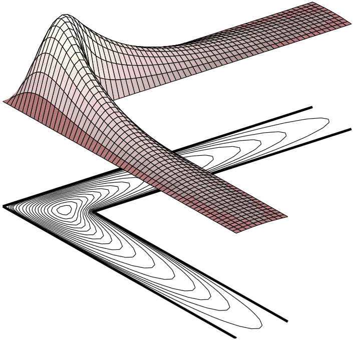
However, for a 'quantum bobsleigh' the transverse contribution to the energy is *quantized* so it may not be able to 'jump' from one transverse level to another one.

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

What is important, the effect of *geometrically induced binding* is *robust*.

To illustrate this claim, consider Ω 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 ≈ 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

Moreover, the binding effect coming from the geometry of the guide is *not restricted to bends*. For instance, it is not difficult to see that bound states occur if the tube has a local *'bulge'*.

Similar effect can also be seen in more complicated geometries. Consider, for instance, a pair of *parallel Dirichlet strips* of widths d_1, d_2 and suppose they are connected laterally by *window of width a* in the common boundary

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

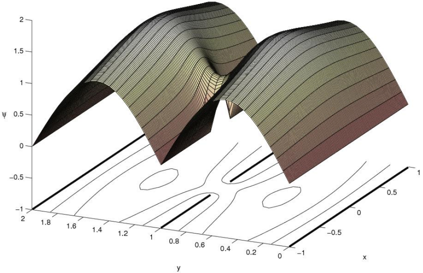
The discrete spectrum of H is nonempty for any $a > 0$ and

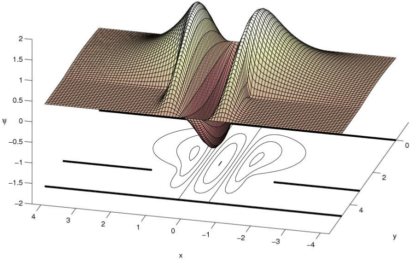
$$\sharp\sigma_{\mathrm{disc}}(H) \geq \frac{2a}{d} \sqrt{1 - \left(\frac{d}{d_1 + d_2}\right)^2}$$

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

Let us plot two eigenfunction, the *ground state* for $d_1 = d_2$ and the *second excited state* is an asymmetric waveguide:





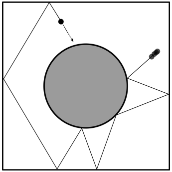
In particular, this example illustrates well the *purely quantum nature* of the effect: a classical particle in such a system *cannot be trapped* except for the (*phase-space measure zero!*) events of reflections, either from the window edges or perpendicular to the walls.

A detour: Šeba billiard

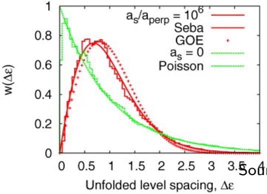
Of course, this is not the only example illustrating *profound differences* between the classical and quantum mechanics. Let us mention one more, remotely related, which concerns a *chaotic behavior*.

In the canonical chaotic behavior example of *Sinai billiard*, shrinking the obstacle to a point, the system becomes *integrable*.

Quantum chaos shows in the *eigenvalue spacing distribution*, and the quantum Sinai billiard *remains chaotic* even if the obstacle is a *point interaction* – for the moment we leave aside what this means. What is important, such an effect was also *observed experimentally*.



Source: wikipedia



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*.

J.T. Londergan, J.P. Carini, D.P. Murdock: *Binding and Scattering in Two-Dimensional Systems. Applications to Quantum Wires, Waveguides and Photonic Crystals*, Springer LNP m60, Berlin 1999.

- Similar results hold for other boundary conditions *except Neumann*. However, if the boundaries are different, the orientation matters, e.g., in a DN strip a bending produces bound states if the Dirichlet condition is *'inside'* and it *does not* in the opposite case.

J. Dittrich, J. Kříž: Curved planar quantum wires with Dirichlet and Neumann boundary conditions, *J. Phys. A: Math. Gen.* **35** (2002), L269–275.

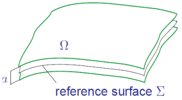
- Similar results hold for three-dimensional bent tubes of *circular cross section*.
- If the cross section *is not circular*, we have to consider the *twisting* which, in contrast to the bending, produces a *repulsive* interaction.

For many more results see

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

Quantum layers

If we take this exercise *one dimension higher*, we can observe other interesting phenomena. Such situations have again a physical meaning, say, as models of electrons is semiconductor *layers on a non-flat substrate*.



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

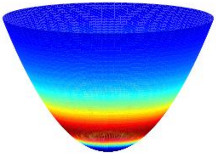
$$H = -\frac{\partial^2}{\partial u^2} - g^{-1/2}\frac{\partial}{\partial s_\mu} g^{1/2} g^{\mu\nu} \frac{\partial}{\partial s_\nu} + K - M^2 + \mathcal{O}(a),$$

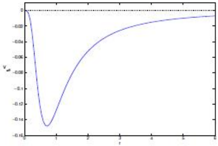
where g is *metric tensor* of the surface Σ, and K, M are its *Gauss* and *mean* curvatures, respectively. Since $K = k_1 k_2$ and $M = \frac{1}{2}(k_1 + k_2)$, the leading term of the effective potential, $K - M^2 = -\frac{1}{4}(k_1 - k_2)^2$, is again of the *attractive* nature, vanishing only on *planes*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

The effective potential in a thin layer

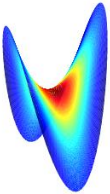
Effective Potential $V_{\text{eff}} = -\frac{1}{4}(k_+ - k_-)^2$

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

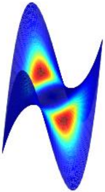




Hyperbolic Paraboloid $z = x^2 - y^2$



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



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

Curvature induced bound states in layers

However, the existence results are not limited to thin layers only:

Theorem

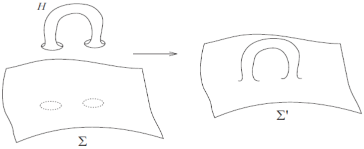
If the surface Σ is C^4 smooth non-planar and $\mathcal{K} = \int_\Sigma K \, \mathrm{d}\Sigma \le 0$ we have $\inf \sigma(H) < \kappa_1^2$. If Σ is asymptotically flat [leaving out again the precise formulation], the the Dirichlet Laplacian has at least one isolated eigenvalue below κ_1^2.

P. Duclos, P.E., H. Krejčiřík: Bound states in curved quantum layers, *Commun. Math. Phys.* **223** (2001), 13–28.

Furthermore, the *Cohn-Vossen inequality* states that

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

where h is the *genus* of Σ and e is the *number of ends*



Nontrivial topology & positive Gauss curvature

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

Theorem

Conclusions of the previous theorem hold whenever Σ is not conformally equivalent to the plane.

G. Carron, P.E., D. Krejčiřík: Topologically non-trivial quantum layers, *J. Math. Phys.* **45** (2004), 774–784.

In the opposite situation, $\mathcal{K} > 0$, we do not have such a universal result, just several *sufficient conditions*. As you may expect, one of them guarantees the existence of curvature induced bound states provided *the layer halfwidth a is small enough*.

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 π built over *conical surface* of an opening angle $\pi - 2\theta$ for some $\theta \in (0, \frac{1}{2}\pi)$,

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

Call the corresponding Dirichlet Laplacian H_θ. We have

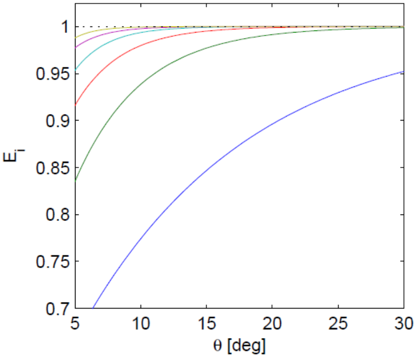
Theorem

For any fixed $\theta \in (0, \frac{1}{2}\pi)$ we have $\sigma_{\rm ess}(H_\theta) = [1, \infty)$ while the discrete spectrum of the operator is non-empty with $\sharp\sigma_{\rm disc}(H_\theta) = \infty$. Each eigenfunction is axially symmetric, i.e. independent of ϕ.

P.E., M. Tater: Spectrum of Dirichlet Laplacian in a conical layer, *J. Phys. A: Math. Theor.* **43** (2010), 474023.

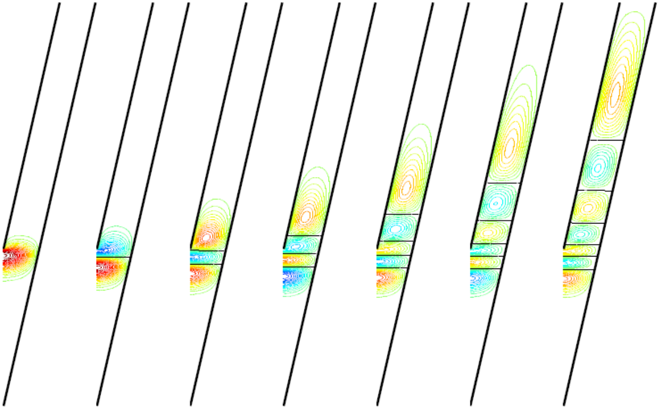
The discrete spectrum infiniteness is related to the fact that the *geodetic circles* on Σ_θ are *shorter* than their counterparts in the plane, which means that the effective attractive potential that behaves asymptotically as $\frac{c}{r^2}$.

Conical layer eigenvalues



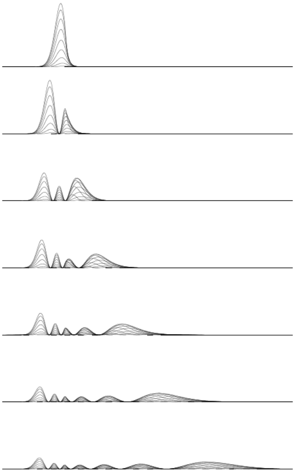
Plot of the dependence of the first six eigenvalues on θ

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 $\theta = \frac{5\pi}{36}$

What to bring home from Lecture I

- A novel concept, such as the one of a quantum graph, is likely to develop rapidly if it reflects a topic *of wide interest in physics*. If it is connected with *attractive mathematical problems*, the better.
- Quantum graphs offer a nice illustration of the *importance of self-adjointness*, or more specifically, they show that this property is much more than mere 'Hermiticity' of operators supposed to represent observables.
- 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.