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Geometrically induced spectral properties of physical systems

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Geometrically induced spectral properties of physical systems

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Abstract

The thesis is aiming at mathematical studies of spectral problems, coming both from modern as well as classical physics, where the significant features of geometry as regards physical properties play a crucial role. We focus on the properties of the nodal set of eigenfunctions and low-lying eigenvalues of vibrating systems, on the influence of curvature and torsion on spectral properties of curved quantum-waveguide nanostructures, on the heat flow in twisted tubes and on the influence of intrinsic curvature on quantum transport on manifolds.

Mathematically, we deal with a spectral-geometric analysis on bounded and quasi-cylindrical domains or, more generally, on non-compact non-complete Riemannian manifolds. The main achievements are represented by the proof of the nodal-line conjecture for a large class of non-convex and possibly multiply connected domains and the establishment of Hardy-type inequalities in twisted tubes and negatively curved surfaces.

0 Introduction

The study of relations between geometry and spectral analysis constitutes an important domain of mathematical physics. Already from a purely mathematical point of view, it is interesting to understand the influence of the shape or metric of a manifold and the type of boundary conditions to the spectra of associated differential operators; and vice versa, one can try to characterize intrinsic properties of a manifold from given spectral data. The physical interest comes from the fact that many systems in Nature are described by partial differential equations, and the latter are often studied by means of a spectral analysis of the corresponding differential operators.

Moreover, eigenvalues and eigenfunctions of the spectral problems usually have direct physical interpretations, and estimating these less accessible quantities on the basis of more accessible geometrical data may already be of a practical interest for the engineer or the physicist.

A typical example is the spectral problem for the Laplace operator in a Euclidean domain. This is a usual model for stationary states of a vibrating object in acoustics and of certain waves in electromagnetism (the Helmholtz equation), or for bound states of a quantum particle constrained to a nanostructure in quantum physics (the stationary Schrödinger equation). It is also related to the stochastic motion of a Brownian particle (the simplest version of the Fokker-Planck equation) and to other diffusive processes. However, apart from very simple symmetric situations where one can employ a separation of variables, no explicit formulae for solutions are available. But the geometry of real systems can be rather complicated, and it is necessary to develop alternative methods of spectral theory in order to provide rigorous information about the spectrum.

The goal of the present thesis is to contribute to this vast area of mathematical physics by analysing the interplay between the geometry and spectrum in the following problems, coming both from classical as well as modern physics:

1. vibrating systems and the nodal-line conjecture,
2. twisting versus bending in waveguide-like structures,
3. quantum mechanics on curved manifolds.

***ad* 1.** Historically, probably the first study of spectral-geometric relationship can be associated with the work of Lord Rayleigh on vibrating systems from the second half of the 19th century. His textbook, *The Theory of Sound* [32], is still referred to by acoustic engineers today and has led to a number of interesting mathematical conjectures, some of them being solved much later or still open. An example of the latter is the famous conjecture of L. E. Payne's from 1967 [30], which states that the nodal line of any second eigenfunction of the Dirichlet Laplacian in an arbitrary planar domain touches the boundary.

Our contribution to this problem is both positive and negative. First, in [FK3], we show that the nodal-line conjecture actually does not hold for unbounded domains. Second, in [FK4], we establish the validity of the conjecture for thin curved tubes (of arbitrary cross-section and in any dimension). It is for the first time when the conjecture has been proved for non-convex domains without any symmetry conditions.

In addition to the aforementioned analysis of nodal set of eigenfunctions, we obtain new isoperimetric-type estimates for low-lying eigenvalues of the Dirichlet Laplacian in star-shaped domains [FK5] and study the instability of solutions to the damped wave equation in possibly unbounded domains [FK1].

***ad* 2.** Waveguide is a physical device (usually of tubular shape) that exhibits propagating states: electromagnetic or acoustic waves in the context of classical physics, or scattering states in quantum mechanics. Mathematically, one deals with the so-called quasi-cylindrical domains, for which the spectral analysis is most difficult because of the presence of both eigenvalues and continuous spectrum. Here the interest in the interplay between the geometry and spectrum for such systems is mainly due to the advent of nanotechnology in the second half of the 20th century. Modern experimental techniques make it possible to fabricate tiny semiconductor structures (often called nanostructures) of various shapes devised and reproducible in the laboratory and yet small enough to exhibit quantum effects, some of them being of purely geometric origin.

Probably the most beautiful phenomenon is the existence of curvature-induced bound states in quantum waveguides, mathematically first described by P. Exner and P. Šeba in 1989 [13]. This paper initiated extensive theoretical studies of waveguide-like objects in quantum mechanics and the research field is still active today, partly because of the advent of new structures such as carbon nanotubes and graphenes. Our contribution to the study of the effect of *bending* in waveguides consists mainly in generalizing the results to higher dimensions [CDFK] and to more general boundary conditions [KK1, FK2, K3] and in applying new mathematical methods in the analysis of scattering states [KT].

However, a genuine breakthrough in the theory is represented by our paper [EKK], in which we observe that the geometric deformation of *twisting* leads to a completely opposite effect in quantum waveguides, mathematically described by the existence of Hardy-type inequalities. Surprisingly, the effect of twisting has been overlooked for almost two decades. We also prove a variant of our original result in a different geometrical setting [KK2] and apply the Hardy-type inequalities to diffusive processes [KZ1, KZ2].

***ad* 3.** The ambient manifold of a quantum waveguide is usually identified with the flat Euclidean space. This restriction is obviously due to the semiconductor-physics motivation, however, at least from the mathematical point of view, one may be interested equally in the situations when it is a general Riemannian manifold. Moreover, this more general setting leads to an interesting conceptual question: *Which geometry is better to travel in?* Or, more precisely, what is the effect of ambient curvature on quantum transport?

We have analysed the problem in the simplest non-trivial case when the ambient space of the quantum traveller is a tubular neighbourhood of an infinite curve in a two-dimensional (abstract) Riemannian manifold. Our principal results can be roughly summarized as follows: positive curvature hurts the transport [K1], while negative curvature improves it [K2]. Mathematically, the former follows as a consequence of the existence of discrete eigenvalues for the Laplace-Beltrami operator, while the latter is based on Hardy-type inequalities. The results have important consequences for the large time behaviour of the Brownian motion [KK3].

The rest of this thesis syllabus consists in a more detailed description of the aforementioned achievements.

1 Vibrating systems

The simplest mathematical model for a vibrating membrane with fixed edge is the wave equation

$$\partial_t^2 u - \Delta_x u = 0 \tag{1}$$

in a planar domain Ω, subject to the Dirichlet boundary condition $u = 0$ on $\partial\Omega$. The eigenfunctions u_n and eigenvalues λ_n of the associated spectral problem

$$\begin{cases} -\Delta u = \lambda u & \text{in } \Omega\,, \\ \quad\; u = 0 & \text{on } \partial\Omega\,, \end{cases} \tag{2}$$

are modes and squared frequencies of vibrations, respectively. The zero set of an eigenfunction corresponds to stationary points of the membrane vibrated in a resonant frequency; it is a curve known as the *nodal line* that forms peculiar shapes (also known as Chladni's patterns): various crossing curves or closed loops.

1.1 The nodal-line conjecture [FK3], [FK4]

It turns out that the shape of the nodal line is related to acoustic properties of the membrane. In particular, it is important to know whether the nodal line of the second eigenfunction u_2 can form a closed loop or not. In this context, the famous conjecture of L. E. Payne's from 1967 [30] states that the nodal line of any second eigenfunction of the Dirichlet Laplacian in an arbitrary bounded two-dimensional Euclidean domain touches the boundary.

So far, it has been shown that the conjecture holds for convex domains [27, 24, 19] and there exist counterexamples with multiply connected domains [21]. Nevertheless, it is still an open question whether the conjecture holds for simply connected domains. Let us also mention that the study of nodal sets of eigenfunctions may of course be extended in a natural way to higher dimensions [25, 14, 26] and manifolds [10, 4, 33, 16].

The positive result [FK4]. In the joint work [FK4] with P. Freitas, we establish the validity of the conjecture in sufficiently thin curved (and therefore non-convex) tubes Ω about curves in Euclidean spaces of arbitrary dimension. We allow for the tube to have an arbitrary cross-section (rotated appropriately with respect to the Frenet frame of the reference curve), and thus we do not exclude the case of multiply connected domains either.

This result may be extended to higher eigenfunctions and we actually show that, given a natural number N greater than or equal to two, for any $2 \leq n \leq N$ the nodal set of the n-th eigenfunction u_n divides the tube Ω into precisely n subdomains, and the closure of each of these subdomains has a non-empty inter-section with $\partial\Omega$, provided that the diameter of the cross-section of Ω is sufficiently small. Moreover, we locate the nodal set near the zeros of the solution of an ordinary differential equation which is associated to the tube in a natural way, via the geometry of the reference curve.

In addition to the fact that we support the validity of the conjecture by a large class of not-previously-considered domains, also our methodological approach to the problem is new. Indeed, our results are based on a resolvent-type convergence of the Dirichlet Laplacian in the tube Ω to a Schrödinger operator on the reference curve. The technical problems due to the fact that we actually deal with a highly singular perturbation (the operators act on Hilbert spaces of different dimensions and the spectrum of the Dirichlet Laplacian explodes in the limit) are overcome by an appropriate identification of the Hilbert spaces and a suitable renormalization of the Laplacian. Finally, we also need to apply methods known from elliptic regularity theory in a scale of Sobolev spaces and to use the maximum principle in a refined way.

In the end of our paper [FK4], we extend the results to the Laplace-Beltrami operator in tubular neighbourhoods of curves on two-dimensional Riemannian manifolds.

The negative result [FK3]. In the other joint paper [FK3] with P. Freitas, we show that the restriction to bounded domains in the nodal-line conjecture is crucial. Indeed, if one does not require the domain to be bounded, then the nodal line need not touch the boundary even under the same assumptions that have been previously used in the bounded case to prove the conjecture. More precisely, we prove that there exists a simply-connected unbounded planar domain Ω which is convex and symmetric with respect to two orthogonal directions, and for which the nodal line of a second eigenfunction does not touch the boundary $\partial\Omega$. This domain can be chosen as one of the following two types (see Figure 1):

(i) the distance between the nodal line of a second eigenfunction and the boundary $\partial\Omega$ is bounded away from zero, but the spectrum of the Dirichlet Laplacian is not purely discrete;

(ii) the spectrum consists only of discrete eigenvalues, but the infimum of the distance between a point on the nodal line of a second eigenfunction and the boundary $\partial\Omega$ is zero.

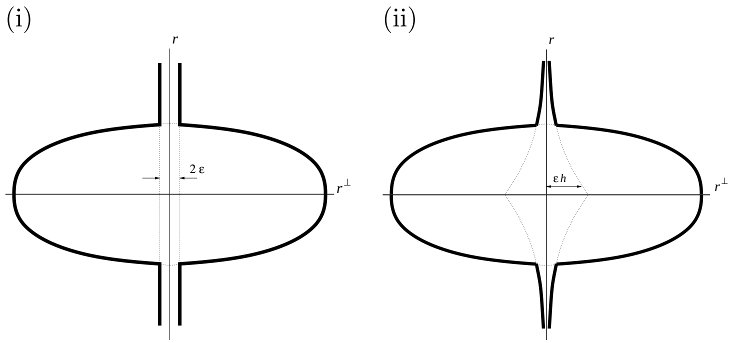

Figure 1: Typical domains for which the nodal line of the second eigenfunction does not touch the boundary.

The idea behind both examples is to start from a bounded convex domain Ω_0 which is invariant under reflections through two orthogonal lines r and $r^{\perp}$, and which we will assume to be sufficiently long in the direction $r^{\perp}$, such that its second eigenvalue is simple and any corresponding eigenfunction is antisymmetric with respect to r. In fact, its second nodal line will be given by the closure of $\Omega_0 \cap r$. We then append two sufficiently thin semi-infinite strips to Ω_0 in neighbourhoods of the points where its second nodal line touches the boundary, in such a way that the nodal line coincides with the axis r and thus stays within these strips without touching the boundary.

In order to establish case (i), we consider domains which are asymptotically cylindrical. This means that there also exists essential spectrum, and so it is necessary to prove that the domain does indeed possess a second discrete eigenvalue in this case. In order for condition (ii) to be satisfied, we consider domains which are asymptotically narrow and thus, although the nodal line does not touch the boundary, it does get asymptotically close to it.

It should be stressed that while the nodal line in both our examples does not touch the boundary, it is not closed.

1.2 The isoperimetric inequalities [FK5]

Among all drums of given area, the circular drum is the one which produces the deepest bass note. This is a musical interpretation of the famous Faber-Krahn inequality (conjectured already by Lord Rayleigh in 1877 [32] but proved almost thirty years later, simultaneously and independently by G. Faber and E. Krahn). Mathematically, in any dimension,

$$\lambda_1(\Omega) \geq \lambda_1(B)\,, \tag{3}$$

where $\lambda_1(\Omega)$ is the first eigenvalue of the Dirichlet Laplacian in a bounded domain Ω and B is the ball having the same volume as Ω. Modulus a set of zero capacity, equality in (3) is attained if and only if Ω is the ball B and it is thus of interest to understand how strong this connection is. In particular, if the domain Ω is *far away* from B, must its first Dirichlet eigenvalue be much larger than that of the ball?

This particular question was given a positive answer respectively in [20] and [28, 2, 17], where the measure of deviation of the domain from the ball which was used was based respectively on the support function of the domain and the Fraenkel asymmetry (*i.e.* Hausdorff distance if Ω is convex).

In the joint paper [FK5] with P. Freitas, we consider the issue of whether having a large first Dirichlet eigenvalue implies being away from the corresponding ball. The main result of this paper in this direction is the following estimate using the isoperimetric constant as a measure of deviation of convex Ω from B:

$$\frac{|\partial\Omega|}{|\Omega|^{1-1/d}} \;\geq\; \frac{|\partial B|}{|B|^{1-1/d}} \sqrt{\frac{\lambda_1(\Omega)}{\lambda_1(B)}} \, \frac{\pi}{2\sqrt{\lambda_1(B_1)}}\,, \tag{4}$$

where B_1 is the d-dimensional ball of unit radius. This bound is, in a sense, optimal for d-dimensional parallelepipeds.

The proof of (4) is based on the (sharp) inequality

$$\lambda_1(\Omega) \;\leq\; \lambda_1(B_1)\, \frac{|\partial\Omega|}{d\,\rho_\Omega\,|\Omega|}\,, \tag{5}$$

where ρ_Ω is the inradius of Ω. (5) is in turn a consequence of a stronger upper bound for $\lambda_1(\Omega)$, holding in the more general case of star-shaped domains, that we establish by using trial functions with mutually homothetic level sets. The stronger bound depends on the support function of the domain Ω in a non-elementary way (therefore we do not present it here) and it is in fact an extension to arbitrary dimensions of an upper bound for $\lambda_1(\Omega)$ appearing in G. Pólya and G. Szegö's 1951 book [31] in the planar case.

As a by-product, we also obtain sharp upper bounds for the second eigenvalue $\lambda_2(\Omega)$ and spectral gap $\lambda_2(\Omega) - \lambda_1(\Omega)$ of convex domains.

1.3 The damped wave equation [FK1]

The wave equation (1) is of course an idealization, since it does not take into account dissipation which always exists in real vibrating systems. A more realistic mathematical model is given by the *damped wave equation*

$$\partial_t^2 u + a(x)\,\partial_t u - \Delta_x u = 0\,. \tag{6}$$

Here the positive part of the damping term a corresponds to a dissipation, while negative "damping" models a supply of energy into the system. Apart from viscoelasticity, (6) models a variety of evolution processes in other areas of physics: electromagnetism (the telegraph equation), relativistic quantum mechanics, cosmology (the Klein-Gordon equation in a curved space-time), *etc.* The indefinite damping also arises after linearizing semilinear damped wave equations around a stationary solution.

In the case where the damping a remains non-negative, the asymptotic behaviour of solutions of (6) is well understood [35]. However, the situation is much less clear in the case of the indefinite damping, precluding the usage of standard energy methods.

In 1991, G. Chen *et al.* [5] conjectured that for bounded intervals and under certain extra conditions on the damping the trivial solution of (6) would remain stable. This was disproved in 1996 by P. Freitas [15], who showed that in the case of bounded domains Ω this sign-changing condition is sufficient to cause the existence of unbounded solutions of (6), provided that the supremum norm of the damping is large enough.

Heuristically, this behaviour can be understood from the fact that, when the sign-changing a is replaced by αa and the parameter α increases, equation (6) (formally) approaches a backward-forward heat equation. Thus one does expect the appearance of complex eigenvalues μ of the associated (operator pencil) spectral problem

$$\begin{cases} -\Delta u + \mu\, a\, u = -\mu^2 u & \text{in } \Omega\,, \\ \qquad\qquad\quad u = 0 & \text{on } \partial\Omega\,, \end{cases} \tag{7}$$

on the positive side of the real axis (which then give rise to unbounded solutions). On the other hand, and still at the heuristic level, note that while for bounded domains the result is not unexpected from the point of view of geometric optic rays either, for unbounded domains this is not as clear.

The lack of results for unbounded domains and/or indefinite damping was a motivation for another joint paper [FK1] with P. Freitas, in which we establish the *instability* of solutions to the wave equation with large (non-homogeneous but time-independent) indefinite damping in (possibly unbounded) domains. Our approach is to reconsider (7) as a spectral problem for a linear albeit non-self-adjoint operator in a Hilbert-space setting and apply some semiclassical-type results for Schrödinger operators in order to establish the existence of spectrum with positive real part

In fact, the main idea behind the results is the same as that used by P. Freitas in [15], however, the generalization is not straightforward because of the presence of essential spectrum for unbounded domains. Moreover, we work under very mild regularity assumptions about the coefficients of a generalized form of (6) and without any restrictions on the geometry of Ω.

2 Quantum waveguides

The evolution of the wavefunction ψ of an effectively free quantum particle confined to a nanostructure with hard walls is described by the Schrödinger equation (in suitable units)

$$i\partial_t\psi = -\Delta_x\psi \tag{8}$$

in a spatial domain Ω, subject to the Dirichlet boundary condition $\psi = 0$ on $\partial\Omega$. The spectral problem associated with (8) formally coincides with (2), however, the interpretation of the spectral quantities is different: the eigenfunctions u_n represent quantum bound states and the corresponding eigenvalues λ_n are their energies.

For unbounded domains Ω, the energy spectrum is not exhausted by eigenvalues, since there is typically also continuous spectrum, which in turn decomposes into absolutely and singularly continuous spectra (the former corresponding to propagating/scattering states and the latter without physical interpretation). This is precisely what happens for *quantum waveguides* modelled by Ω being unbounded tubular neighbourhoods of curves in the three-dimensional Euclidean space (see Figure 2).

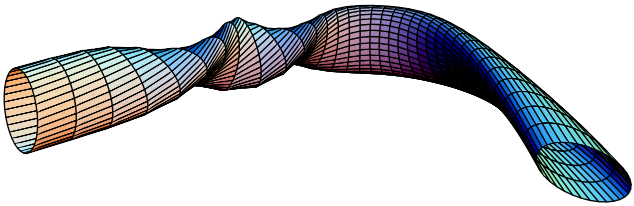

Figure 2: An example of a waveguide of elliptical cross-section. Twisting and bending are demonstrated on the left and right part of the picture, respectively.

Let us remark that the spectral problem for the Laplacian in tubular domains is relevant in other areas of physics as well (electromagnetic and acoustic waveguides, fluid dynamics, *etc*).

2.1 The effect of bending [CDFK]

It turns out that the energy spectrum is extremely sensitive to geometric deformations of the quantum waveguide. It is probably best demonstrated by an astonishing 1989 result of P. Exner and P. Šeba [13], who demonstrated the existence of discrete eigenvalues in *bent* two-dimensional strips. A generalization to three-dimensional tubes with circular cross-section was done in [18, 11]. The result is indeed far from being obvious, because the quantum bound states do not have classical counterparts (more precisely, it is a wave effect).

In the joint work with B. Chenaud, P. Duclos and P. Freitas [CDFK], we ask the question whether the phenomenon of the existence of bound states in bent quantum waveguides continues to exist, first, for higher-dimensional tubes and, second, for tubes of general (*i.e.* non-circular) cross-sections. After generalizing the geometric concept of curved waveguides to higher dimensions, we successfully extend the standard variational proof of the existence of discrete spectrum to tubes whose (arbitrary) cross-section is "appropriately" rotated along the reference curve with respect to the Frenet frame. Moreover, we present a new proof of the location of the essential spectrum, which does not require any conditions whatsoever about the derivatives of curvature.

2.2 The effect of twisting [EKK, KK2]

The above paper [CDFK], in which we study the effect of bending in quantum waveguides of arbitrary cross-section, does not answer the question what happens with the spectrum (in particular with the discrete eigenvalues) if the cross-section is *not* appropriately rotated along the reference curve with respect to the Frenet frame, so that the tube is also *twisted* (see Figure 2). The effect of twisting is more subtle, because the twist itself (*i.e.* no bending) does not change the spectrum, and more refined functional-analytic techniques are required to describe it. This is probably the reason why the spectral consequences of twisting in quantum waveguides had not been discovered until our breakthrough contribution [EKK].

In this joint work with T. Ekholm and H. Kovařík [EKK], we actually prove the existence of *Hardy-type inequalities* in twisted waveguides. More precisely, we show that the functional inequality

$$\int_\Omega |\nabla\psi|^2 - E_1 \int_\Omega |\psi|^2 \geq \int_\Omega \frac{|\psi(x)|^2}{1+|x|^2}\, dx \tag{9}$$

holds true for all ψ in the Sobolev space $H_0^1(\Omega)$ if, and only if, the waveguide is locally twisted (no bending). Here E_1 denotes the threshold of the essential spectrum (coinciding with the first Dirichlet eigenvalue in the cross-section). Consequently, twisting acts as an repulsive interaction and the spectrum of a twisted waveguide is stable against small (attractive) perturbations.

Furthermore, we employ the inequality (9) in order to show that the spectrum is stable against geometric deformations as well: a simultaneously twisted and mildly bent waveguide does not possess discrete eigenvalues. Putting it somewhat popularly, this result provides a prescription for experimentalists on how to produce bound-state-free waveguide nanostructures.

In the follow-up work with H. Kovařík [KK2], we show that the effect of twisting is robust by establishing an analogous Hardy-type inequality in a two-dimensional waveguide twisted via boundary conditions (see Figure 3).

Figure 3: Twisting in a two-dimensional strip introduced via switching Dirichlet (thick lines) to Neumann (thin lines) boundary conditions at one point, and *vice versa*.

2.3 More general boundary conditions [KK1, FK2, K3]

As we have already mentioned, the Dirichlet boundary condition $\psi = 0$ represents hard-wall boundaries, which are used to model large chemical barrier on the interface between two semiconductor materials. However, it is not the most general condition modelling impenetrable walls of Ω. A more general boundary condition, which ensures that there is no probability current through the boundary $\partial\Omega$, is given by Robin-type boundary conditions

$$\frac{\partial\psi}{\partial n} + \alpha\psi = 0 \qquad \text{on} \qquad \partial\Omega\,, \tag{10}$$

where $\alpha : \partial\Omega \to \mathbb{R}$ and n denotes the outward unit normal to $\partial\Omega$. The extreme cases $\alpha = 0$ and $\alpha = +\infty$ correspond to Neumann and Dirichlet boundary conditions, respectively. The other values of α may in principle be relevant for different types of interface in a solid and it is thus important to understand the interplay between the boundary conditions, geometry and spectral properties.

In the joint work with J. Kříž [KK1], we make a comparative study of the situation of a planar strip with Dirichlet, Neumann and a combination of these boundary conditions. It turns out that the existence of bound state is highly sensitive to the nature of boundary conditions imposed: there is always discrete spectrum in locally curved Dirichlet strips, there is no for Neumann strips and, most interestingly, the existence of bound states in strips with Dirichlet condition on one boundary curve and Neumann on the other depends on the direction to which the strip is bent. The last phenomenon was observed for the first time by J. Dittrich and J. Kříž in 2002 [9]. In addition to an extensive study of the existence and properties of bound states by means of variational methods, we give a new proof of the location of the essential spectrum in quantum waveguides, which does not require any conditions whatsoever about the decay of derivatives of curvature at infinity.

In order to explain the peculiar spectral properties of the strip with a combination of Dirichlet and Neumann boundary conditions (the model of [9]) established in [KK1, 9] by the variational proofs, in the follow-up work [K3], we derive two-term (semiclassical type) asymptotics for the eigenvalues in the limit when the strip width tends to zero.

Finally, in the joint work P. Freitas [FK2], we consider a more general situation when the Neumann boundary condition is replaced by a variable Robin boundary condition. We prove that, for certain α, the spectral threshold of the associated Laplacian is estimated from below by the lowest eigenvalue of the Laplacian in a Dirichlet-Robin annulus determined by the geometry of the strip. Moreover, we show that an appropriate combination of the geometric setting and boundary conditions leads to a Hardy-type inequality in the infinite strips. As an application, we derive certain stability of the spectrum for the Laplacian in Dirichlet-Neumann strips along a class of curves of sign-changing curvature, improving in this way an initial result of J. Dittrich and J. Kříž [9].

2.4 Nature of the essential spectrum [KT]

In analogy with the spectra of atoms, the energy spectrum of a locally curved quantum waveguide typically consists of the interval $[E_1, \infty)$ representing the continuous (or, more precisely, essential) spectrum and of a number of discrete eigenvalues below E_1. In principle, the structure of the essential spectrum can be quite complex: apart from the absolutely continuous part (representing propagating states), there might be embedded eigenvalues (bound states) and also a (physically obscure) singularly continuous spectrum. For scattering theory, it is important to know that the singularly continuous spectrum is not present and to have a control over the embedded eigenvalues.

In the joint work with R. Tiedra de Aldecoa [KT], we make a thorough analysis of the essential spectrum of locally bent but untwisted waveguides of arbitrary cross-section in any dimension. Under suitable assumptions about the decay of curvatures at infinity, we prove that the singularly continuous spectrum is empty and that the set of eigenvalues is closed and countable, with possible accumulation points only at the thresholds given by the discrete set of Dirichlet eigenvalues of the cross-section. A limiting absorption principle follows as a consequence of the results.

In addition to the generalizations to any dimensions and to waveguides of arbitrary cross-section, the results of the paper [KT] provide, in comparison with previous results established in [12] by different methods, alternative sufficient conditions to ensure the important spectral properties. An analogous analysis of the essential spectrum for twisted but unbent three-dimensional tubes was made only recently in [3].

Our analysis is based on Mourre conjugate operator method developed for acoustic multistratified domains in [1, 8]. As a technical preliminary, we carry out a spectral analysis for general Schrödinger-type operators in straight tubes. We also apply the general result to strips embedded in abstract surfaces.

2.5 Diffusive processes [KZ1, KZ2]

It is well known that some quantum properties (*e.g.* regularity of bound states, criticality of the Hamiltonian, *etc*) are better studied by considering the heat semigroup associated with the Hamiltonian instead of the Schrödinger unitary group. In the quantum-waveguide context, this consists in replacing (8) by the heat equation

$$\partial_t u - \Delta_x u = 0 \tag{11}$$

(formally obtained by considering imaginary times in (8)). Moreover, (11) models diffusive processes in other areas of physics (*e.g.* heat flow, Brownian motion, *etc*).

In the joint work with E. Zuazua [KZ1], we examine the influence of the existence of the Hardy inequality (9) in twisted waveguides on the *large-time behaviour* of the solutions to (11). First, we give a new proof of the Hardy inequality, which is more elegant than that presented in [EKK] and holds under less restrictive conditions about the geometry of Ω. Second, we establish a new Nash-type inequality, which holds irrespectively of whether the tube is twisted or not. The latter can be used in energy estimates to derive a robust decay estimate for the solutions of (11), optimal for straight (*i.e.* untwisted) waveguides.

The main objective of the paper [KZ1] is to show that a better decay estimate holds in twisted waveguides, as a consequence of (9). Unfortunately, energy estimates does not seem to be useful and we had to instead apply a refined version of the method of self-similar variables together with the theory of weighted Sobolev spaces in order to show that (9) indeed ends up enhancing the decay rate of the solutions. One version of our main results can be stated in terms of the following inequality

$$\|u(t)\| \leq C\,(1+t)^{-1/4-\gamma}\,e^{-E_1 t}\,\|u_0\|_w\,. \tag{12}$$

Here u_0 denotes the initial datum, $\|\cdot\|_w$ stands for the norm in the weighted space $L^2(\Omega, w(x)\,dx)$ with $w(x) := e^{|x|^2/4}$ and C, γ are constants (independent of u, u_0 and t). Our result says that

γ is (strictly) *positive* if, and only if, the tube Ω is twisted

(otherwise necessarily $\gamma = 0$, and it is easy to see that for straight tubes the inequality (12) with $\gamma = 0$ is optimal). The result can be interpreted as that the twisting implies a faster cool-down/death of the medium/Brownian particle in the tube.

In the follow-up work with E. Zuazua [KZ2], we show similar results, by the same techniques, for the two-dimensional waveguide twisted via boundary conditions, for which the existence of Hardy inequality was established in [KK2].

3 Quantum traveller on manifolds

The problem of quantization on submanifolds of Riemannian manifolds has attracted a considerable attention from the beginning of quantum mechanics, partly because of the frustrating fact that different approaches lead to different results (see [22] for a concise comparison and [34] for a recent review with many references). Apart from a conceptual importance, the problem is motivated by several specific applications, such as molecular dynamics and physics of nanostructures.

A physically reasonable quantization procedure for the latter can be achieved by imposing a large confining potential in the vicinity of a submanifold of the Euclidean space and by the renormalization consisting in throwing away the exploding normal oscillations in the limit when the neighbourhood shrinks. This leads to an effective Hamiltonian that contains information on, *inter alia*, how the submanifold is embedded in the ambient space [23] (so that the result is not really intrinsic).

Performing the same procedure for submanifolds in a *curved ambient space*, one reveals that the effective Hamiltonian additionally depends on the intrinsic curvature of the ambient Riemannian manifold [29]. An interesting conceptual question is how this curvature affects the quantum transport. The problem is equally interesting for other physical models, such as the heat flow or Brownian motion on curved manifolds.

In a series of papers [K1, K2, KK3], we attacked the above question in the simplest non-trivial model when the ambient manifold is an (abstract) surface $\mathcal{A}$ of (Gauss) curvature K (not necessarily embedded in the three-dimensional Euclidean space) and the submanifold is an infinite curve of (geodesic) curvature κ on it. The confining potential is represented by Dirichlet boundary conditions imposed at a fixed (not necessarily small) distance a from the curve.

Hence, we can again think about the spectral problem (2), however, it is important to keep in mind that the strip-like tubular neighbourhood Ω is a manifold now and $-\Delta$ has the meaning of the Laplace-Beltrami operator. Our main strategy to study spectral properties of the operator is to express it in the Fermi (or geodesic parallel) coordinates based on the reference curve (see Figure 4).

3.1 Positive curvature [K1]

In [K1], we start with analysing the effect of positive curvature K of the ambient manifold $\mathcal{A}$. It turns out that the positivity leads to stationary solutions of the Schrödinger equation, hurting in this way the transport in the strip Ω. Let us mention that the presence of bound states was predicted by formal

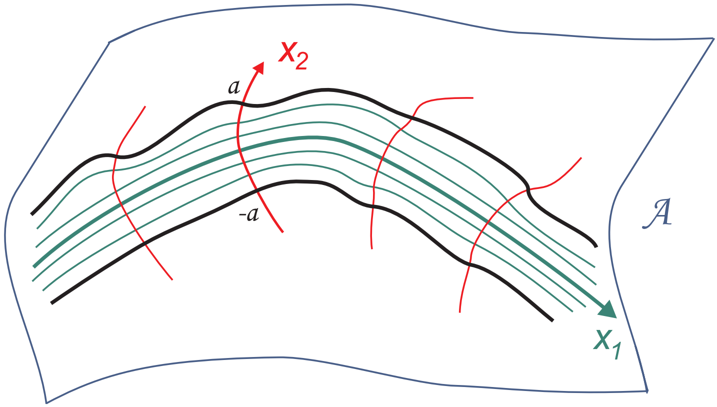

Figure 4: The parameterization of the strip Ω via Fermi coordinates $x = (x_1, x_2)$.

arguments in [7, 6].

More precisely, by a variational test-function argument, we show that the Laplace-Beltrami operator on $L^2(\Omega)$, subject to Dirichlet boundary conditions, possesses discrete eigenvalues below the essential spectrum, provided that K is a non-trivial non-negative function on Ω vanishing at the infinity of the strip. The bound states exist also if K vanishes identically but the geodesic curvature κ is non-trivial and vanishing at the infinity of the strip. The results can be viewed as a generalization of the classical result of P. Exner and P. Šeba [13].

3.2 Negative curvature [K2]

The above paper [K1] does not answer the question what happens with the spectrum (in particular with the discrete eigenvalues) if the curvature is non-positive, although it is conjectured there that the bound states can be eliminated by the presence of negative curvature. Indeed, the effect of negative curvature is more subtle, for similar reasons as the twisting in quantum waveguides (*cf* Section 2.2).

To get at least a partial insight into the problem, in the follow-up paper [K2], we study a special class of negative ambient spaces: *ruled surfaces*. The corresponding strips Ω can be thought as obtained by translating and rotating a segment along a straight line in the three-dimensional Euclidean space (see Figure 5).

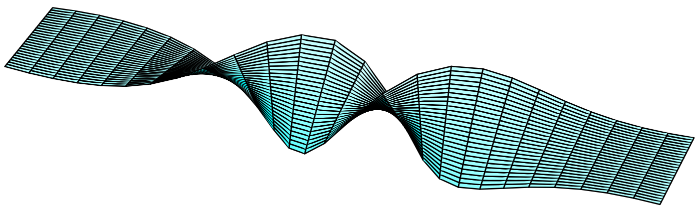

Figure 5: A ruled strip as a twisted ribbon.

First, we establish the existence of Hardy-type inequalities (9) in ruled strips along geodesics (*i.e.* $\kappa = 0$), as a consequence of the presence of negative curvature. Second, we use these inequalities to show that there are no discrete eigenvalues even if the reference curve is a mildly perturbed geodesic, improving in this sense the transport in Ω. The results provide a positive answer to some conjectures raised in [K1].

3.3 Large-time behaviour [KK3]

The objective of the most recent joint work with M. Kolb [KK3] is twofold. First, we establish the existence of Hardy-type inequalities (9) for a larger class of "negatively curved manifolds"; for instance, it is just enough to assume that the strip is negatively curved in a vicinity of the reference curve to have a Hardy-type inequality (9) for small a. Second, we specify the meaning of the "bad" and "good" transport in the positively and negatively curved strips, respectively. Our approach is probabilistic, viewing the traveller in Ω as a Brownian particle governed by (11) and the properties of the transport are interpreted in terms of the large-time behaviour of the solutions u. Roughly speaking, by the "good geometry" for transport we understand that which enables the Brownian traveller to reach his/her goal as soon as possible or "to escape from his/her starting point as far as possible".

If the curvature K is non-trivial non-negative, vanishing at the infinity of the strip, then the existence of the ground-state energy $\lambda_1 < E_1$ implies that the decay rate is slower in comparison with the straight case ($K = 0 = \kappa$). This is as a direct consequence of the (sharp) spectral-type estimate

$$\|u(t)\| \leq e^{-\lambda_1 t} \|u_0\| . \tag{13}$$

On the other hand, the effect of negative curvature is more subtle and, in analogy with the heat equation in twisted waveguides (*cf* Section 2.5), we had to apply the machinery of self-similar variables and weighted Sobolev spaces in order to conclude that (12) holds with *positive* γ whenever there is a Hardy inequality of the type (9). Consequently, if the curvature K is non-trivial non-positive, vanishing at the infinity of the strip, the decay rate is faster in comparison with the straight case.

In addition to the norm-wise estimates (12) and (13), we also establish a number of point-wise results for probability densities.

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