Centre de Physique Théorique* - CNRS - Luminy, Case 907
F-13288 Marseille Cedex 9 - France

CURVATURE–INDUCED BOUND STATES IN QUANTUM WAVEGUIDES IN TWO AND THREE DIMENSIONS

Pierre DUCLOS[1] and Pavel EXNER[2]

Abstract

Dirichlet Laplacian on curved tubes of a constant cross section in two and three dimensions is investigated. It is shown that if the tube is non–straight and its curvature vanishes asymptotically, there is always a bound state below the bottom of the essential spectrum. An upper bound to the number of these bound states in thin tubes is derived. Furthermore, if the tube is only slightly bent, there is just one bound state; we derive its behaviour with respect to the bending angle. Finally, perturbation theory of these eigenvalues in any thin tube with respect to the tube radius is constructed and some open questions are formulated.

October 1994
CPT-94/P.3023

anonymous ftp or gopher: cpt.univ-mrs.fr

*Unité Propre de Recherche 7061
[1]and PHYMAT, Université de Toulon et du Var, 83130 Lagarde, France
duclos@naxos.unice.fr
[2]Nuclear Physics Institute, AS CR, 25068 Řež near Prague
and Doppler Institute, Czech Technical University, Břehová 7, 11519 Prague, Czech Republic
exner@ujf.cas.cz

Contents

1 Introduction

1.1 What are the quantum waveguides?

A rapid development of microelectronics has stimulated in recent years a remarkable progress in semiconductor physics. Many new ideas have appeared and the experimental framework has widened considerably. At the same time this progress has brought interesting mathematical problems but this fact escaped the general attention. The present paper is devoted to some of them.

The most spectacular manifestation of the mentioned achievements concern fabrication techniques of microscopic structures of a pure semiconductor material – see, *e.g.*, [Sa] and the papers quoted below. Let us recall some of them:

(i) thin films produced on an insulating surface by one of the epitaxial techniques; their thickness can be as small as $2\,nm$ which means that the transversal cross section of such a layer contains several atoms only,

(ii) sandwiches obtained by combining films of different semiconductor materials; a typical example is the combination of GaAs and AlGaAs,

(iii) heterostructures, *i.e.*, sandwiches with a variating layer thickness – see, *e.g.*, [DB],

(iv) *"quantum wires"* obtained from semiconductor films by suitable masking and ion bombardment – see [TDP]; in this way one can create on the substrate various graphs,

(v) similarly one can produce many–probe junctions like the structures investigated in [TBV, Ba] *etc.*

One often uses the term *mesoscopic physics* for experiments with such structures and other similarly small objects (like, for instance, metallic graphs prepared by ion lithography). The goal is to stress that the systems involved are large enough to be shaped by the experimentalist and at the same time so small that quantum effects like interference are manifested on them. Among the experimental achievements made in this field, recall the manifestation of Aharonov–Bohm effect in heterostructures [DMB] and metallic rings [BLD, UHL, WWU]; some other experiments will be mentioned later. Recall also that the quantum interference in microstructures controlled by an external field is of a considerable interest: there are several proposals of interference transistors [DB, EŠ3, SMRH] which surpass by their size, speed and switching voltage the commonly used MOSFETs.

Let us summarize characteristic properties of the mentioned semiconductor microstructures: they are

(a) small size, typically from tens to hundreds of nm,

(b) high purity; the electron mean free path can be a few μm or even larger,

(c) crystallic structure,

(d) the wavefunctions are usually suppressed at the boundaries between different semiconductor materials – see, *e.g.*, [HH].

Behaviour of an electron in such a structure is, of course, governed by the many–body Schrödinger equation describing its interaction with the lattice atoms including possible impurities. The mentioned properties allow us, however, to adopt several fundamentally simplifying assumptions.

It is obvious from (a) and (b) that using a sufficiently pure material one can achieve that the mean free path is two or three orders of magnitude greater than the size of the structure; hence the electron motion can be assumed in a reasonable approximation as undisturbed by the scattering on impurities. Experimentalists are used to speak about a ballistic regime, and they are able to prove it, for example, by measuring interference effects which are excluded under other circumstances.

The property (c) allows us to make the most important simplification. It is well known that a particle in a crystallic lattice moves as *free* with some effective mass m^*; from the mathematical point of view it follows from spectral properties of Schrödinger operators with periodic potentials – see [RS], Sec.XIII.16. The effective mass changes, of course, along the spectrum but one can regard it as a constant when we restrict our attention to the physically interesting part of the valence band. Recall that its value may differ substantially from the true electron mass, for instance, one has $m^* = 0.067\, m_e$ for GaAs.

In combination with (d) we see that the electron motion inside the microstructure can be modelled by a free (spinless) particle living in the corresponding spatial region with the *Dirichlet condition* on its boundary; an interaction term must be added only if the whole structure is placed into an external field.

Investigation of quantum motion in a fixed subset of the configuration space represented until recently rather a textbook illustration, and nearly nothing was known concerning complicated regions like curved or branched tubes, layers or sandwiches. The new developments in semiconductor physics discussed above offer a strong motivation for studying of such systems; in view of the natural analogy and also for the sake of brevity we shall refer to them as to **quantum waveguides**.

Introducing such a notion, one is naturally compelled to ask about the relations to the classical theory of acoustic and electromagnetic waveguides (the literature devoted to these problems is rather extensive; let us name [CJ, Go, KLR, KRS, KRT], [Marc, Me] as a few examples related in a way to the subject of the present paper). The basic equations in the two cases, *i.e.*, the Schrödinger and wave equation are, of course, different but as far as one is concerned with the stationary problems only, both of them reduce to the Helmholz equation in the appropriate spatial region. The difference is then in the physical meaning of the spectral parameter, and possibly also in the boundary conditions which are Neumann for the acoustic and EM–mode of the electromagnetic waveguides (in the quantum case, one can encounter the Neuman conditions when considering ballistic motion of electrons in metallic microstructures).

This means that some results of the classical theory can be easily adapted to the quantum case. On the other hand, quantum mechanics and the classical theory of waves use rather different mathematical methods so a mutual inspiration could be useful on both sides. For instance, the results discussed below can be used to establish existence of trapping modes in bent electromagnetic waveguides with perfectly conducting walls which was not suspected in the classical theory [EŠ2].

1.2 Subject of the paper and survey of results

Let us specify first the scope of the paper. The quantum waveguide theory, though it exists up to now in a very rudimentary form only, offers a lot of interesting problems. In this paper, we are going to concentrate to those related to the *curvature–induced discrete spectrum* of the corresponding Hamiltonian *in bent tubes*.

As we have mentioned, the existence of square–integrable solutions to the wave equation remain unnoticed in the classical theory of waveguides. In quantum mechanics, several authors [dC1, dC2, dC3, Pi, JK, KJ, Ma] presented independently formal considerations (aimed mostly at the quantization problem for motion on curves and surfaces) which contained implicitly the existence of bound states. One can find also other indications for existence of the effect, for example, the numerical solution to Schrödinger equation on the oval–shaped ring [SRS] which demonstrates that the wavefunction is localized to the regions of maximum curvature.

The effect was clearly recognized for the first time in the paper [EŠ1] where the Birman–Schwinger technique in combination with the minimax principle was used to demonstrate that the Dirichlet Laplacian on a smooth curved planar strip which is thin enough and whose curvature decays sufficiently rapidly has at least one isolated eigenvalue below the bottom of the essential spectrum. The analogous result was proved in [E2] for curved tubes in $\mathbb{R}^3$; the decay assumption has been later substantially weakened [E3], and some lower bounds to the bound–state energies were derived [AE].

Another considerable progress was achieved in [GJ] (see also [DJ]) where a suitably chosen trial function was used to demonstrate that any bending pushes the threshold of the spectrum below the lowest transverse–mode energy; this implies the existence of bound states in curved tubes of any thickness provided the curvature is zero outside a bounded region, or at least vanishes asymptotically.

Though all these results apply to smooth tubes of a constant cross section, analogous results are valid also in similar geometries. An example was given in [EŠŠ1] showing that bound states can exist in a sharply broken L–shaped strip; the computed bound–state energy has been verified experimentally in a flat electromagnetic waveguide in [CLM1] (an early mathematical treatment of this effect can be found in [He]). Other examples of this type are given, *e.g.*, in [ABGM, CLM2, SRW]. As for physical consequences of curvature–induced bound states, in addition to the trapping modes already mentioned, *e.g.*, the existence of edge–confined currents in thin semiconductor films was conjectured [EŠŠ2] and a model of resonance scattering in finite–length quantum wires was analyzed [E1].

The present paper is devoted to a review and a further development of ideas formulated in the above mentioned papers. In the next two sections we discuss bent tubes in $\mathbb{R}^2$ and $\mathbb{R}^3$, respectively. Following the idea of [GJ], we prove the existence of bound states in a curved tube under not very strong assumptions about the regularity of the boundary and the decay of the curvature. Using a trick known from Schrödinger operator theory [Kl, New, Se] we are able to derive here also an upper bound to the number of bound states in sufficiently thin tubes in terms of the tube curvature.

In the three–dimensional case one has to know also the torsion of the generating curve to characterize the tube. For simplicity, we consider mostly cylindrical tubes but we specify also a more general class to which the results extend easily. Apart from this, the torsion is much less important for the existence of bound states; all we need it that it satisfies some weak regularity assumptions.

It is certainly not easy to compute the bound–state energies directly, and therefore perturbation theory is of natural interest. In Sections 4 and 5 we treat the eigenvalues in bent tubes perturbatively with respect to two different parameters. First we study mildly curved tubes replacing the curvature γ by $\gamma_\beta := \beta\gamma(\cdot)$. The parameter β is proportional to the tube bending angle. If it is small enough, the corresponding Dirichlet Laplacian has just one simple eigenvalue; we compute the gap between it and the threshold of the continuous spectrum in terms of β.

Another natural perturbative parameter is the tube radius a. In Section 5 we compare the tube Hamiltonian H to a simple operator in which the transverse and longitudinal variables are decoupled, and the discrete spectrum is given explicitly in terms of the discrete spectra of the "component" operators. We find that for thin enough tubes there is a bijective correspondence between this spectrum and the discrete spectrum of H, and show that an asymptotic expansion in terms of a exists up to any prescribed order; the perturbation series for the eigenvalues is computed. We also show that the mode–coupling terms in the Hamiltonian begin to contribute at the fourth order in a only, and discuss an alternative in which H is compared to a suitable operator family.

We conclude the paper by showing several open problems and directions in which the results obtained here could be further extended. Physics of quantum waveguides attracts nowadays a lot of attention; recently a wave of papers has appeared containing results on different levels of rigor, often numerical, concerning the curvature–induced bound states [ABGM, WSM1, WS] as well as those coming from bulges and crossings [SRW, WSMK, IN, NI], geometrically induced resonances and the associated transport problem [VOK1, VOK2, WS] *etc.*

2 A strip in the plane

2.1 Preliminaries

Consider a curved strip Ω in $I\!\!R^2$ of a constant width $d=2a$, and choose its axis as the reference curve Γ. Up to Euclidean transformations, Ω is uniquely characterized by a and the function $s\mapsto\gamma(s)$, where s is the arc length of Γ and γ is the (signed) curvature. We assume that

(r1) $\gamma\in L^1_{loc}(I\!\!R)$,

(r2) $a\|\gamma\|_\infty<1$,

(r3) Ω is not self–intersecting.

Sometimes it is useful to consider strips with a large winding angle, then the last assumption can be avoided by a slight generalization: instead of a plane we consider a strip on a multi–sheeted Riemannian surface.

We are interested in the Dirichlet Laplacian (*cf.* [RS], Sec.XIII.15) $-\Delta_D^\Omega$ on the strip, excluding the trivial case of a straight Ω. As in [EŠ1], one can introduce locally orthogonal coordinates s,u ; the operator $-\Delta_D^\Omega$ is then unitarily equivalent to

$$\tilde H\;=\;-g^{-1/2}\,\partial_s\,g^{-1/2}\partial_s\;-\;g^{-1/2}\,\partial_u\,g^{1/2}\partial_u \tag{1}$$

on $L^2(I\!\!R\times(-a,a),\,g^{1/2}ds\,du\,)$ with the Dirichlet condition at $u=\pm a$, where $\partial_s:=\partial/\partial s$, *etc.*, and $g^{1/2}(s,u):=1+u\gamma(s)$ is the corresponding Jacobian. If γ is not smooth, the operator $\tilde H$ has to be understood in the form sense. Under a stronger regularity assumption, namely

(r4) γ is piecewise C^2 with $\dot\gamma,\,\ddot\gamma$ bounded

we can pass to another unitarily equivalent operator,

$$H\;=\;-\partial_s\,(1+u\gamma)^{-2}\,\partial_s\;-\;\partial_u^2\;+\;V(s,u) \tag{2}$$

on $L^2(I\!\!R\times(-a,a)\,)$ with

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

which is *e.s.a.* on $D(H) = \{\psi : \psi \in C^\infty,\ \psi(s,-a) = \psi(s,a) = 0,\ H\psi \in L^2\}$.

The above listed regularity assumptions cover various classes of operators. We shall concentrate on the case where Ω is curved substantially within a bounded region only, *i.e.*, the curvature obeys suitable decay assumptions, *e.g.*,

(d1) $\gamma, \dot\gamma\ \ddot\gamma \in L^\infty_\varepsilon(I\!\!R)$,

(d2) $\gamma, \dot\gamma \in L^2(I\!\!R, |s|\, ds)$, and $\ddot\gamma \in L^1(I\!\!R, |s|\, ds)$;

recall that $L^\infty_\varepsilon(I\!\!R)$ is the set of L^∞ functions with the property that to any $\varepsilon > 0$ there is a compact K_ε such that $\|f \upharpoonright K_\varepsilon\|_\infty < \varepsilon$. Since the functions involved are bounded, *(d2)* strengthens *(d1)*. The latter requires $\lim_{|s|\to\infty} \gamma(s) = 0$, while *(d2)* corresponds for a purely powerlike asymptotics of γ to an $\mathcal{O}(|s|^{-1-\varepsilon})$ decay; an easy integration shows that the borderline refers in the last case to a logarithmic–spiral asymptotics of Γ.

2.2 Existence of bound states

The most general existence result is a consequence of the following theorem the basic idea of which belongs to Goldstone and Jaffe [GJ].

2.1 Theorem. *Assume (r1)–(r3). If the strip is not straight, i.e.,* $\gamma \neq 0$, *then* $\inf \sigma(-\Delta_D^\Omega) < \kappa_1^2$, *where* $\kappa_1 = \pi/2a$. *In particular, if* $\inf \sigma_{ess}(-\Delta_D^\Omega) = \kappa_1^2$, *then* $-\Delta_D^\Omega$ *has at least one isolated eigenvalue of finite multiplicity.*

Proof. The argument is based on a variational estimate. Denote the norm in $L^2(I\!\!R \times (-a,a),\, g^{1/2} ds\, du)$ as $\|\cdot\|_g$; then it follows from (1) that

$$q[\Phi] := \|\tilde H^{1/2}\Phi\|_g^2 - \kappa_1^2\|\Phi\|_g^2 = \|g^{-1/4}\partial_s\Phi\|^2 + \|g^{1/4}\partial_u\Phi\|^2 - \kappa_1^2\|g^{1/4}\Phi\|^2 \quad (4)$$

holds for any Φ in $Q(\tilde H)$, the quadratic form domain of $\tilde H$, where $\|\cdot\| := \|\cdot\|_1$. In particular, choosing $\Phi(s,u) := \varphi(s)\chi_1(u)$, where $\chi_1(u) := \sqrt{\frac{2}{d}}\,\cos(\kappa_1 u)$ is the lowest transverse–mode function, we find

$$q[\Phi] = \|\langle g^{-1/4}\rangle\dot\varphi\|^2_{L^2(I\!\!R)},$$

where $\langle\cdot\rangle$ means the expectation with respect to χ_1. It is clear that it is sufficient to find $\Phi \in D(\tilde H)$ for which $q[\Phi]$ is negative.

Let $K := [-c,c]$ for some $c > 0$ and choose the function φ from the Schwartz space $\mathcal{S}(I\!\!R)$ in such a way that $\varphi(s) = 1$ on K. Furthermore, we define the family $\{\varphi_\lambda : \lambda \in I\!\!R\}$ by a scaling exterior to K:

$$\varphi_\lambda(s) := \begin{cases} \varphi(s) & \ldots \quad |s| \le c \\ \varphi(\pm c + \lambda(s \mp c)) & \ldots \quad \pm s > c \end{cases} \quad (5)$$

It is easy to check that

$$q[\Phi_\lambda] \;\le\; \|\langle g^{-1/2}\rangle\|_\infty^2 \|\dot\varphi_\lambda\|^2 \;\le\; \frac{\lambda}{1-a\|\gamma\|_\infty}\,\|\dot\varphi\|^2 \tag{6}$$

holds for $\Phi_\lambda :\; \Phi_\lambda(s,u) \,=\, \varphi_\lambda(s)\chi_1(u)$, so $q[\Phi_\lambda]$ can be made arbitrarily small by choosing λ small enough.

Next we pick $j \in C_0^\infty(K\times(-a,a))$ and set $\phi := j^2(\tilde H - \kappa_1^2)\Phi_\lambda$. For non–zero $\gamma,\, j$ this vector is non–zero; one can compute explicitly

$$\phi(s,u) \,=\, -\left(j^2\,\frac{\gamma}{1+u\gamma}\,\partial_u\chi_1\right)(s,u) \,=\, j^2(s,u)\sqrt{\frac{2}{d}}\,\frac{\kappa_1\gamma(s)}{1+u\gamma(s)}\,\sin(\kappa_1 u)\,.$$

Recall that γ is non–zero as an element of L^1_{loc} if there is a compact set (without loss of generality, it may be identified with K) such that $\int_K |\gamma(s)|\,ds \ne 0$. Then $\gamma\ne 0$ also in $L^2_{loc}(I\!R)$ because $\int_K |\gamma(s)|\,ds \le |K|^{1/2}\left(\int_K |\gamma(s)|^2\,ds\right)^{1/2}$, and therefore $\phi\ne 0$ as an element of $L^2(I\!R\times(-a,a))$. Since both Φ_λ and ϕ belong to $D(\tilde H)$, we have

$$q[\Phi_\lambda+\varepsilon\phi] \,=\, q[\Phi_\lambda] \,+\, 2\varepsilon\|j(\tilde H-\kappa_1^2)\Phi_\lambda\|^2 \,+\, \varepsilon^2(\phi,(\tilde H-\kappa_1^2)\phi)\,,$$

where the second term on the right side does not depend on λ because the scaling acts out of the support of the localization function j. For all sufficiently small negative ε the sum of the last two terms is negative, and we can choose λ so that $q[\Phi_\lambda+\varepsilon\phi] < 0$. ∎

This result implies that the discrete spectrum of $-\Delta_D^\Omega$ is non–empty provided the bending does not push the essential–spectrum threshold down; this happens typically if the curvature decays to zero at infinity. In particular, we have the following result.

2.2 Corollary. *Let a curved strip satisfy the assumptions (r1)–(r3). Any of the conditions*

(a) γ *has a compact support,*

(b) (r4) and (d1)

is sufficient for $-\Delta_D^\Omega$ *to have at least one bound state of energy below* κ_1^2.

Proof. In the first case we can choose s_0 in such a way that the cuts of the strip at $s=\pm s_0$ are outside of the curved part. We impose there the Neumann condition; this turns $\tilde H$ into the orthogonal sum $\tilde H_N = \tilde H_- \oplus \tilde H_0 \oplus \tilde H_+$. The spectrum of the middle part is purely discrete while the tail operators have a purely continuous spectrum, so $\sigma_{ess}(\tilde H_N) = \sigma_{ess}(\tilde H_- \oplus \tilde H_+) = \sigma(\tilde H_- \oplus \tilde H_+) = [\kappa_1^2,\infty)$. On the other hand, we have $\tilde H_N \le \tilde H$ (*cf.* [RS], Sec.XIII.15), so the result follows by the minimax principle.

Under the strengthened regularity assumption *(r4)*, we may pass to the unitarily equivalent operator (2). This makes it possible to use known results of the theory of Schrödinger operators, since the latter can be estimated by

$$H_{\pm} \,:=\, -\,(1 \mp a\|\gamma\|_{\infty})^{-2}\partial_s^2 \,-\, \partial_u^2 \,+\, V \tag{7}$$

or more roughly by

$$\hat{H}_{\pm} \,:=\, -\,(1 \mp a\|\gamma\|_{\infty})^{-2}\partial_s^2 \,-\, \partial_u^2 \,+\, \hat{V}_{\pm}(s)$$

with $\hat{V}_{\pm} := \pm \sup\{\pm V(s,\cdot) :\; u \in (-a,a)\,\}$. The sought result follows from the last mentioned estimate, since $V_{\pm} \in L^{\infty}_{\varepsilon}$ due to *(d1)*, so $\inf \sigma_{ess}(\hat{H}_{\pm}) = \kappa_1^2$ and the same is, of course, true for H. ∎

The part (a) corresponds to the situation treated in [GJ]. As an element of $L^2(I\!\!R \times (-a,a))$, the trial function used in the proof of the theorem is $(s,u) \mapsto \sqrt{1+u\gamma}\,(\Phi_{\lambda} + \varepsilon\phi)$. It is clearly better than the one of Lemma 3.6 in [E3] because it yields the existence of eigenvalues for *any* strip width.

2.3 Thin strips: number of bound states

Minimax estimates of the above mentioned type are useful in many ways. As the first illustration, we shall use them to derive an upper bound to the number of bound states supported by a curved strip which is thin enough.

2.3 Proposition. *Assume (r1–4) and (d2), and furthermore, let*

$$a \,<\, \frac{c_2}{1 + c_2\|\gamma\|_{\infty}}\,,$$

where

$$c_2 \,:=\, \min\left\{ \frac{\pi}{\|\gamma\|_{\infty}}\,,\, \left(\frac{\pi^2}{2\|\ddot{\gamma}\|_{\infty}}\right)^{1/3}\,,\, \left(\frac{\pi}{\sqrt{5}\|\dot{\gamma}\|_{\infty}}\right)^{1/2} \right\}\,,$$

then the number $N(H)$ of isolated eigenvalues (counting multiplicity) obeys

$$N(H) \,\le\, 1 \,+\, \frac{1}{8}\left(\frac{1 + a\|\gamma\|_{\infty}}{1 - a\|\gamma\|_{\infty}}\right)^2\, \frac{\int_{I\!\!R^2} \gamma(s)^2|s-t\,|\gamma(t)^2\,ds\,dt}{\int_{I\!\!R}\gamma(s)^2\,ds}\,. \tag{8}$$

Proof. We estimate H from below by

$$H \,\ge\, H_{-} \,:=\, \overline{(1 + a\|\gamma\|_{\infty})^{-2}\; h_{-} \otimes I \,+\, I \otimes G}$$

with

$$h_{-} \;:=\; -\,\frac{d^2}{ds^2} \,+\, (1 + a\|\gamma\|_{\infty})^2\, V_{-}(s)\,,$$

$$V_{-}(s) \;:=\; -\,\frac{\gamma^2}{4(1 - a\|\gamma\|_{\infty})^2} \,-\, \frac{a\|\ddot{\gamma}\|_{\infty}}{2(1 - a\|\gamma\|_{\infty})^3} \,-\, \frac{5}{4}\,\frac{a^2\|\dot{\gamma}^2\|_{\infty}}{(1 - a\|\gamma\|_{\infty})^4}$$

and G denoting $-\partial_u^2$ on $L^2(-a,a)$ with Dirichlet b.c. In view of the assumption, the modulus of each term of $V_-(s)$ is $\le \pi^2/4a^2$, and therefore only the lowest eigenvalue of G can contribute to $\sigma_d(H_-)$. Hence we have $N(H) \le N(H_-) \le N(h_-)$. Moreover, the two last terms in the potential $(1+a\|\gamma\|_\infty)^2\, V_-(s)$ are s–independent so $N(h_-) = N(\tilde h_-)$, where

$$\tilde h_- \,:=\, -\,\partial_s^2 \,-\, \frac{1}{4}\left(\frac{1+a\|\gamma\|_\infty}{1-a\|\gamma\|_\infty}\right)^2 \gamma(s)^2\,,$$

and the known bound [Kl, New, Se] yields the result. ∎

In particular, we get a sufficient condition under which a thin strip has just one bound state; roughly speaking, this happens if Ω has one simple bend, *i.e.*, γ is sign–preserving and has one well distinguished peak – *cf.* [E2]. In Chapter 4 below we shall see that the same is true for any Ω which satisfies the assumptions of Corollary 2.2(b) provided it is only slightly bent.

3 A tube in $I\!R^3$

Now we apply the same ideas to a three–dimensional quantum waveguide.

3.1 "Straightening" of a curved cylindrical tube

Let $\Gamma \in C^k(I\!R, I\!R^3)$, $k \ge 2$, be a curve and (T,B,N) the corresponding Frenet triad frame. Given $a>0$, we denote $B_a := \{\, x \in I\!R^2 \,:\, |x| < a\,\}$ and define $f \,:\, I\!R \times B_a \to \Omega$ by

$$f(s,r,\theta) \,:=\, \Gamma(s) \,-\, r\,[\,N\,\cos(\theta-\alpha) \,+\, B\,\sin(\theta-\alpha)\,]\,,$$

where the function $\alpha \,:\, I\!R \to I\!R$ will be chosen later. If γ, τ are the curvature and torsion of Γ, respectively, one has the Frenet formula

$$\partial_s \begin{pmatrix} T \\ N \\ B \end{pmatrix} = \begin{pmatrix} 0 & \gamma & 0 \\ -\gamma & 0 & \tau \\ 0 & -\tau & 0 \end{pmatrix} \begin{pmatrix} T \\ N \\ B \end{pmatrix}$$

Since the vectors $N,\, B$ express in terms of $\dot\Gamma,\, \ddot\Gamma$ (the dots always mean differentiation with respect to s), $f \in C^{k-2}$. Let us compute the Jacobian matrix $f' := Jf$.

$$\partial_s f \,=\, T\,(1+r\gamma\,\cos(\theta-\alpha)) \,-\, r(\dot\alpha-\tau)N\,\sin(\theta-\alpha) \,-\, r(\tau-\dot\alpha)B\,\cos(\theta-\alpha)$$

$$\partial_r f \,=\, -N\,\cos(\theta-\alpha) \,-\, B\,\sin(\theta-\alpha)$$

$$\partial_\theta f \,=\, rN\,\sin(\theta-\alpha) \,-\, rB\,\cos(\theta-\alpha)$$

so one has immediately

$$|g| := |f'|^2 := \det(Jf)^2 = r^2\,(1 + r\gamma\,\cos(\theta-\alpha))^2$$

with

$$g := {}^t\!f' f' = \begin{pmatrix} (1 + r\gamma\,\cos(\theta-\alpha))^2 & 0 & r^2(\tau-\dot\alpha)^2 \\ 0 & 1 & 0 \\ r^2(\tau-\dot\alpha)^2 & 0 & r^2 \end{pmatrix}$$

Hence we have proven

3.1 Lemma. *Suppose* $\alpha \in C^{k-2}$ *and* $a\|\gamma\|_\infty < 1$, *then* f *is a local* C^{k-2} *diffeomorphism. It becomes global if* f *is required to be injective.*

3.2 The images of $-\Delta_D^\Omega$

The described change of variables provides us with two distinct operators which are unitarily equivalent to $-\Delta_D^\Omega$. Let first $\tilde H$ be the image of $-\Delta_D^\Omega$ under $\tilde U : L^2(\Omega) \to L^2(I\!R\times B_a, |g|^{1/2} ds\, dr\, d\theta)$ defined by $\tilde U\Phi := \Phi\circ f$; it is straightforward to check that

$$\tilde H = |g|^{-1/2}\nabla^*|g|^{1/2}g^{-1}\nabla\,,$$

where ∇ means the gradient operator in the variables (s, r, θ) and $\nabla^* := -\mathrm{div}$. The most simple situation occurs if we choose

$$\dot\alpha = \tau\,, \tag{9}$$

because g is then diagonal and the transformed operator does not contain mixed derivatives between the longitudinal and transversal coordinates; notice that the corresponding rotating coordinate frame is known in the classical waveguide theory under the name of Tang coordinate system [TG]. With this choice we get

$$\|\tilde H^{1/2}\Phi\|_g^2 = \|r^{1/2}|g|^{-1/4}\partial_s\Phi\|^2 + \||g|^{1/4}\partial_r\Phi\|^2 + \||g|^{1/4}r^{-1}\partial_\theta\Phi\|^2\,, \tag{10}$$

for any $\Phi \in Q(\tilde H)$ and the subscript g refers to the metric as in (4).

The other representation of $-\Delta_D^\Omega$ is obtained by the unitary mapping $U : L^2(\Omega) \to L^2(I\!R\times B_a)$ defined by $U\Phi = |f'|^{1/2}\Phi\circ f$. A simple calculation yields the identities

$$H := U(-\Delta_D^\Omega)U^{-1} = |g|^{-1/4}\nabla^*|g|^{1/2}g^{-1}\nabla|g|^{-1/4} = \nabla^* g^{-1}\nabla - \frac{(\nabla^* g^{-1}(\nabla|g|^{1/4}))}{|g|^{1/4}}\,,$$

where the last term has to be understood as a multiplication by the corresponding function. Using again the Tang coordinate system, we arrive at the formula

$$H = -\partial_s h^{-2}\partial_s - \Delta_{B_a} + V(s, r, \theta)\,, \tag{11}$$

where

$$h \,:=\, 1 + r\gamma\, \cos(\theta - \alpha)\,,$$

$-\Delta_{B_a} := -\partial_r^2 - r^{-2}\partial_\theta^2 - \frac{1}{4} r^{-2}$ with the Dirichlet b.c. and

$$V(s,r,\theta) \,=\, |g|^{-1/4}(\nabla^* g^{-1}(\nabla |g|^{1/4})) \,+\, \frac{1}{4} r^{-2}\,.$$

To express the "effective potential" V in a more explicit form, we employ the relations

$$\begin{aligned} h_s \,&:=\, r\gamma\tau\, \sin(\theta - \alpha) \,+\, r\dot\gamma\, \cos(\theta - \alpha)\,, \\ h_{ss} \,&:=\, r(\ddot\gamma - \gamma\tau^2)\, \cos(\theta - \alpha) \,+\, r(2\dot\gamma\tau + \gamma\dot\tau)\, \sin(\theta - \alpha) \end{aligned}$$

which allow us to write

$$V(s,r,\theta) \,=\, -\,\frac{\gamma^2}{4h^2} \,+\, \frac{1}{2}\,\frac{h_{ss}}{h^3} \,-\, \frac{5}{4}\,\frac{h_s^2}{h^4}\,. \tag{12}$$

Notice that the *lhs* of (12) is similar to the "two–dimensional potential" (3). In particular, their expansions in powers of r, u, respectively, have the same structure which makes it possible to develop the perturbation theory simultaneously for the two cases.

3.2 Remarks. (a) As in the two–dimensional case, $-\Delta_D^\Omega$ is the Friedrichs extension of the operator L which acts as Laplacian on $D(L) \,=\, C_0^\infty(\Omega)$ (*cf.* [RS], Sec.XIII.15). The form domain of $-\Delta_D^\Omega$ is $\mathcal{H}_0^1(\Omega)$, and moreover, since $\partial\Omega$ has the segment property, $\{\, g \in C^\infty(\Omega) \,:\, g = 0 \;\text{ on }\; \partial\Omega \,\}$ is a core for $-\Delta_D^\Omega$. Consequently, the operator H with $Q(H) = \mathcal{H}_0^1(I\!\!R \times B_a)$ is the Friedrichs extension of $\dot H_0 \,:=\, U\dot L U^{-1}$ defined on $C_0^\infty(I\!\!R \times B_a)$, and furthermore

$$D \,:=\, \{\, u \in C^\infty(I\!\!R \times B_a) \,:\, u(s,a,\theta) = 0 \;\text{ for all }\; s,\, \theta \,\}$$

is a core for H. The same reasoning applies to the operator $\tilde H$.
(b) It is easy to express the operator H using the Cartesian coordinates $x = r\cos\theta,\; y = r\sin\theta$ in the transversal plane. In particular, for $\dot\alpha = 0$ one recovers the results of [Pi].
(c) In the same way one can treat a non–cylindrical tube replacing B_a by the corresponding open connected set G in the transversal plane. If Ω is obtained by moving G along Γ rotating it simultaneously with respect to the Frenet triad frame with the angular velocity $\dot\alpha = \tau$, then one has only to replace $-\Delta_{B_a}$ by the Dirichlet Laplacian $-\Delta_G$. In the general case when (9) is no longer valid, the operators $\tilde H$ and H contain mixed derivatives; we are not going to consider this case in the present paper.

3.3 Existence of bound states

In the three-dimensional case the regularity assumptions look as follows:

(r1) $\gamma,\, \tau \in L^1_{loc}(I\!\!R)$,

(r2) $a\|\gamma\|_\infty < 1$,

(r3) the map $f\,:\, I\!\!R \times B_a \to \Omega$ defined above is injective.

This allows us to pass to the operator $\tilde{H}$ defined above; however, if the functions $\gamma,\,\tau$ are not smooth enough the latter has to be understood in the form sense. As in the previous chapter, we shall also use an additional requirement, namely:

(r4) τ is piecewise C^1, γ is piecewise C^2 with $\gamma,\,\dot\gamma,\,\ddot\gamma$ and $\tau,\,\dot\tau$ bounded,

Under this assumption, we have right to use the operator (11).

We shall again consider again only tubes whose curvature is in some sense localized, *e.g.*,

(d1) $\gamma,\,\dot\gamma,\,\ddot\gamma \in L^\infty_\varepsilon(I\!\!R)$.

We shall also need a stronger hypothesis which involves suitable decay restrictions on the torsion:

(d2) $\gamma,\,\dot\gamma$ and $\tau,\,\dot\tau$ belong to $L^2(I\!\!R, |s|\,ds)$, and $\ddot\gamma \in L^1(I\!\!R, |s|\,ds)$,

Comparing to the two–dimensional case, however, one can take now various combinations of decay requirements on the curvature and torsion to get the needed fall–off of the effective potential. It is even possible to consider the curves Γ whose torsion does not decay at all assuming

(d2') $\gamma,\,\dot\gamma,\,\ddot\gamma \in L^1(I\!\!R, |s|\,ds)$;

the price we pay is, of course, a stronger requirement on the decay of γ. The basic existence result reads as follows.

3.3 Theorem. *Assume (r1)–(r3). If the tube is not straight, i.e.,* $\gamma \ne 0$, *then* $\inf\sigma(-\Delta_D^\Omega) < \inf\sigma(-\Delta_{B_a})$. *In particular, if* $\inf\sigma_{ess}(-\Delta_D^\Omega) = \inf\sigma(-\Delta_{B_a})$, *then* $-\Delta_D^\Omega$ *has at least one isolated eigenvalue of a finite multiplicity.*

Proof. It is customary to number eigenvalues of $-\Delta_{B_a}$ starting from $N = 0$; the lowest one is κ_0^2, where $\kappa_0 := j_{0,1}a^{-1}$ with $j_{0,1}$ being the lowest zero of the Bessel function J_0. Let χ_0 be the eigenfunction corresponding to κ_0^2; then

$$\int_{B_a} r\,dr\,d\theta\, \left(|\partial_r\chi_0|^2 - \kappa_0^2|\chi_0|^2\right) \,=\, 0$$

and an easy integration by parts shows that

$$\int_{B_a} r^2 dr\, d\theta\, \left(|\partial_r \chi_0|^2 - \kappa_0^2 |\chi_0|^2 \right) \,=\, 0\,.$$

Next we choose $\Phi(s,r,\theta) := \varphi(s)\chi_0(r)$, where φ is an arbitrary function of $\mathcal{S}(I\!\!R)$. Using then (10), we get

$$q[\Phi] \,:=\, \|\tilde{H}^{1/2}\Phi\|_g^2 \,=\, \|\langle r^{1/2}|g|^{-1/4}\rangle \dot{\varphi}\|^2_{L^2(I\!\!R)}\,,$$

where as before $\langle\cdot\rangle$ means the expectation with respect to χ_0. The rest of the argument is completely analogous to that of Theorem 2.1. ∎

As in the two–dimensional case, we have

3.4 Corollary. *Let a curved tube satisfy the assumptions (r1)–(r3). Any of the conditions*

- *(a)* γ *has a compact support,*
- *(b) (r4) and (d1)*

is sufficient for $-\Delta_D^\Omega$ *to have at least one bound state of energy below* κ_0^2.

3.4 Thin tubes: number of bound states

Using a minimax estimate of the type (7), one can prove

3.5 Proposition. *Assume (r1–4) and (d2) or (d2'), and furtheremore, let*

$$a \,<\, \frac{c_3}{1+c_3\|\gamma\|_\infty}\,,$$

where

$$c_3 \,:=\, \min\left\{ \frac{\sqrt{10}}{\|\gamma\|_\infty},\, \left(\frac{5}{\|\gamma\tau^2-\ddot{\gamma}\|_\infty + \|2\dot{\gamma}\tau+\gamma\dot{\tau}\|_\infty} \right)^{1/3},\, \left(\frac{\sqrt{2}}{\|\gamma\tau\|_\infty + \|\dot{\gamma}\|_\infty} \right)^{1/2} \right\}\,,$$

then the number of eigenvalues (counting multiplicity) fulfils the inequality (8).

Proof. The lowest two eigenvalues of $-\Delta_{B_a}$ are $\kappa_0^2 := \kappa_{01}^2 = 5.78\, a^{-2}$ and $\kappa_{11}^2 = 14.68\, a^{-2}$. We estimate H from below as in Proposition 2.2 with

$$\begin{aligned} V_-(s) \,=\, &-\frac{\gamma^2}{4(1-a\|\gamma\|_\infty)^2} \\ &- a\,\frac{\|\gamma\tau^2-\ddot{\gamma}\|_\infty + \|2\dot{\gamma}\tau+\gamma\dot{\tau}\|_\infty}{2(1-a\|\gamma\|_\infty)^3} \,-\, a^2\,\frac{5(\|\gamma\tau\|_\infty + \|\dot{\gamma}\|_\infty)^2}{4(1-a\|\gamma\|_\infty)^4}\,. \end{aligned}$$

Under the assumption, modulus of each term is $< \frac{5}{2}a^{-2}$ so the higher transversal modes do not yield isolated eigenvalues, and one can proceed as in the two–dimensional case. ∎

Notice that the torsion enters the bound (8) only through the range of a for which this relation is valid. This is connected with the fact that for a thin tube Ω the spectral properties are given primarily by the curvature of Γ as we shall see in Chapter 5.

4 Bound states in mildly curved tubes

Now we want to discuss the case of tubes of any thickness which are only slightly bent. To this end, we need a parametrization which would allow us to compare different tubes. Among various possibilities we choose the simplest one; we shall consider families of generating curves Γ_β characterized by the curvature

$$\gamma_\beta(s) := \beta\gamma(s) \tag{13}$$

for a fixed function γ and $\beta > 0$. Since the integral of the curvature over an interval $[s_1, s_2]$ is the angle between the tangent vectors to Γ_β at the corresponding points, it is clear that the parameter β controls bending of the tube.

We have seen that in the three–dimensional case it is the curvature and not torsion which is responsible for the existence of non–empty discrete spectrum; hence we limit ourselves to families of tubes with a scaled γ and τ fixed. One should pay attention to the nature of the straightening which corresponds to the limit $\beta \to 0$. As an illustration, suppose that γ has a compact support; then the length of the curved part remains preserved and the curvature radius at each point grows proportionally to β^{-1}. We have the following general result.

4.1 Theorem. *Assume that the hypotheses (r1)–(r4) and (d2) (or (d2') in the three–dimensional case) are valid. Then for all β small enough, $-\Delta_D^\Omega$ corresponding to the tube generated by Γ_β has exactly one isolated eigenvalue $e(\beta)$. Moreover,*

(a) in the two–dimensional case, its asymptotic behaviour is given by

$$\begin{aligned} \sqrt{\kappa_1^2 - e(\beta)} \;=\; \frac{\beta^2}{8}\Big\{ \|\gamma\|^2 \\ + \frac{1}{2}\sum_{N=2}^{\infty} (\chi_N, u\chi_1)^2 \varrho_N \int_{I\!R^2} \dot\gamma(s)\, e^{-\varrho_N|s-s'|}\dot\gamma(s')\, ds\, ds' \Big\} \;+\; \mathcal{O}(\beta^3)\,, \end{aligned} \tag{14}$$

where $\varrho_N := \kappa_1\sqrt{N^2-1}$; the sum runs in fact over even N only.

(b) Similarly, for a three–dimensional tube we have

$$\sqrt{\kappa_0^2 - e(\beta)} \;=\; \frac{\beta^2}{8}\,\|\gamma\|^2 + \frac{\beta^2}{16}\,\sum_{N=1}^{\infty}\,\varrho_N \int_{B_a\times B_a} d\omega\,d\omega'\chi_0(\omega)\chi_0(\omega')\chi_N(\omega)\chi_N(\omega')$$

$$\times \int_{I\!R^2} ds\,ds' h_s(s,r,\theta)\,e^{-\varrho_N|s-s'|}h_s(s',r',\theta') \;+\; \mathcal{O}(\beta^3)\,, \tag{15}$$

where $h_s \;=\; r\,\gamma\tau\,\sin(\theta-\alpha) + r\,\dot\gamma\,\cos(\theta-\alpha)$ *was introduced in Section 3.2,* $d\omega := r\,dr\,d\theta$ *and* $\varrho_N := \sqrt{\kappa_N^2-\kappa_0^2}$ *with* $\kappa_N^2 = j_{n,m}^2 a^{-2}$ *are the transverse mode energies (properly ordered).*

The formulae (14), (15) have a transparent structure. The first term comes from the attractive potential $-\frac{1}{4}\gamma^2$ which dominates the picture for thin tubes, while the rest expresses the contribution of higher transverse modes (see also Remark 4.3 below).

4.1 Weakly coupled Schrödinger operators in a cylinder

To prove the above theorem, we need an auxiliary result which is of interest independently of the present context.

Let M be an open connected set in $I\!R^{\nu-1}$, $\nu \ge 2$, with $\overline{M}$ compact, and consider the operator

$$H_\lambda \;=\; -\,\Delta_D \;+\; \lambda V$$

on $L^2(I\!R)\otimes L^2(M)$, where $-\Delta_D$ is the Dirichlet Laplacian on $I\!R\times M$ which is closure of $(-d^2/dx^2)\otimes I_{\nu-1} + I_1\otimes(-\Delta_D^M)$, and the potential V is supposed to be *measurable* and *bounded.* The last assumption is made with our aim in mind; it is not difficult to extend the argument presented below to potentials with local singularities.

The Dirichlet Laplacian $-\Delta_D^M$ on $L^2(M)$ has a purely discrete spectrum consisting of eigenvalues $0 < \kappa_0^2 < \ldots < \kappa_N^2 < \kappa_{N+1}^2 < \ldots$; the corresponding normalized eigenvectors will be denoted as χ_{N_j}, $N = 0,1,\ldots$ and $j = 1,\ldots,d_N$. It is known that the lowest eigenvalue is simple, $d_0 = 1$, and χ_0 can be chosen positive ([RS], App. to Sec.XIII.12). Due to the boundedness, the functions

$$V_{mn} \;:=\; \int_M \overline{\chi}_m(y)V(\cdot,y)\chi_n(y)\,dy$$

are again measurable and bounded for any m,n. In analogy with V_{00}, we define $|V|_{00}$ as the ground–state matrix element of the function $|V(\cdot,\cdot)|$.

4.2 Theorem. *Assume that* V *is non–zero and* $|V|_{00} \in L^1(I\!R,|x|\,dx)$ *, then* H_λ *has for small* λ *at most one simple eigenvalue* $e(\lambda) < \kappa_0^2$*, and* *this happens iff* $\int_{I\!R} \lambda V_{00}(x)\,dx \le 0$. *Moreover, if this condition holds the following expansion is valid*

$$\begin{aligned}\sqrt{\kappa_0^2 - e(\lambda)} \;=\; & -\frac{\lambda}{2}\int_{I\!R} V_{00}(x)\,dx \;-\; \frac{\lambda^2}{4}\left\{\int_{I\!R^2} V_{00}(x)|x-x'|V_{00}(x')\,dx\,dx'\right.\\ & \left. -\sum_{N=1}^{\infty}\sum_{j=1}^{d_N}\int_{I\!R^2} V_{0N_j}(x)\,\frac{e^{-\sqrt{\kappa_N^2-\kappa_0^2}|x-x'|}}{\sqrt{\kappa_N^2-\kappa_0^2}}\,V_{N_j0}(x')\,dx\,dx'\right\}\\ & +\mathcal{O}(\lambda^3)\,. \end{aligned} \tag{16}$$

Proof. According to Birman–Schwinger principle, $e(\lambda)$ is a bound state of H_λ *iff* λK_α has eigenvalue -1 for $\alpha^2 = e(\lambda)$ where $K_\alpha := |V|^{1/2}(-\Delta_D - \alpha^2)^{-1}V^{1/2}$ and $V^{1/2} := |V|^{1/2}\mathrm{sgn}\,V$. Since $-\Delta_D^M$ is reduced by the projections P_N to its eigenspaces, $-\Delta_D$ is reduced by $I_1 \otimes P_N$ and the same is true for its resolvent whose kernel equals

$$R_0(\alpha;x,y;x',y') \;=\; \sum_{N=0}^{\infty}\sum_{j=1}^{d_N}\chi_{N_j}(y)\,\frac{e^{-k_N(\alpha)|x-x'|}}{2k_N(\alpha)}\,\overline{\chi}_{N_j}(y') \tag{17}$$

where we have denoted $k_N(\alpha) := \sqrt{\kappa_N^2-\alpha^2}$. The first term in this expansion has a singularity at $\alpha = \kappa_0$ which we want to single out. This can be done by taking $K_\alpha = M_\alpha + L_\alpha$, where

$$M_\alpha(x,y;x',y') \;=\; |V(x,y)|^{1/2}\chi_0(y)\,\frac{e^{-k_0(\alpha)|x-x'|}-1}{2k_0(\alpha)}\,\chi_0(y')V(x',y')^{1/2}$$

as in [EŠ1], which would require $V_{00} \in L^1(I\!R, |x|^2\,dx)$. To get a better result, we replace following [BGS, E3] the above decomposition for $\alpha < \kappa_0$ by $K_\alpha = Q_\alpha + P_\alpha$ with

$$Q_\alpha(x,y;x',y') \;=\; \frac{e^{-k_0(\alpha)|x|}}{2k_0(\alpha)}\,|V(x,y)|^{1/2}\chi_0(y)\,e^{-k_0(\alpha)|x'|}\,\chi_0(y')V(x',y')^{1/2}$$

and $P_\alpha := A_\alpha + |V|^{1/2}B_\alpha V^{1/2}$, where

$$\begin{aligned} & A_\alpha(x,y;x',y')\\ &\quad= \frac{1}{k_0(\alpha)}\,|V(x,y)|^{1/2}\chi_0(y)\,\left[e^{-k_0(\alpha)|x|_>}\sinh k_0(\alpha)|x|_<\right]\,\chi_0(y')V(x',y')^{1/2} \end{aligned} \tag{18}$$

and the kernel of B_α is given by (17) with the summation running over $N = 1,2,\dots$; here we have introduced

$$|x|_< \;:=\; \max\{\,0\,,\min(|x|,|x'|)\,\mathrm{sgn}\,(xx')\,\}$$

and $|x|_> := \max\{|x|, |x'|\}$. It is easy to see that for any $\alpha_0 < \kappa_1$, the norm $\|B_\alpha\|$ has in $[0, \alpha_0]$ a bound independent of α. The norm of A_α can be estimated as follows:

$$\begin{aligned} \|A_\alpha\|^2 &\le \|A_\alpha\|^2_{HS} \\ &\le \int_{I\!R\times M}\int_{I\!R\times M} |V(x,y)\chi_0(y)|^2 |x|^2_< |V(x',y')\chi_0(y')|^2\, dx\, dy\, dx'\, dy' \\ &\le \left(\int_{I\!R} |x|\, |V|_{00}(x)\, dx\right)^2, \end{aligned}$$

where we have employed the inequalities $e^{-z'}\sinh z \le z$ for $z' \ge z$ and $|x|^2_< \le |xx'|$, respectively.

Moreover, by dominated convergence $A_\alpha \to A_{\kappa_0}$ as $\alpha \to \kappa_0$ where the last operator has the kernel $A_{\kappa_0}(x,y;x',y') = |V(x,y)|^{1/2}\chi_0(y)|x|_<\chi_0(y')V(x',y')^{1/2}$, so it is again bounded. Together we see that $\|P_\alpha\|$ has in $[0,\alpha_0]$ a bound independent of α. Then $\|\lambda P_\alpha\| < 1$ holds for small enough λ and we may write

$$(I+\lambda K_\alpha)^{-1} = [I+\lambda(I+\lambda P_\alpha)^{-1}Q_\alpha]^{-1}(I+\lambda P_\alpha)^{-1},$$

hence λK_α has eigenvalue -1 *iff* the same is true for $\lambda(I+\lambda P_\alpha)^{-1}Q_\alpha$. Since Q_α is a rank–one operator, $\lambda(I+\lambda P_\alpha)^{-1}Q_\alpha = (\psi,\cdot)\varphi$ with $\psi := \frac{\lambda}{2k_0(\alpha)}\, e^{-k_0(\alpha)|\cdot|}V^{1/2}\chi_0$ and $\varphi := (I+\lambda P_\alpha)^{-1}e^{-k_0(\alpha)|\cdot|}|V|^{1/2}\chi_0$, it has just one eigenvalue $\xi(\lambda) = (\psi,\varphi)$. Putting it equal to -1 we get for $k_0(\alpha) := z$ the following equation

$$z = G(\lambda, z) \tag{19}$$

where

$$G(\lambda,z) = -\frac{\lambda}{2}\int_{I\!R\times M} e^{-z|x|}V(x,y)^{1/2}\chi_0(y)[(I+\lambda P_{\alpha(z)})^{-1}e^{-z|\cdot|}|V|^{1/2}\chi_0](x,y)\, dx\, dy\,. \tag{20}$$

If V decreases exponentially, G is analytic around $(0,0)$ and the assertion follows by implicit–function theorem; it gives also a prescription how to compute other terms in the expansion (16).

In the general case, more caution is needed. First of all, writing $z(\lambda) = a\lambda + b\lambda^2 + r(\lambda)$ one finds easily that (16) solves again the equation (19), however, now we know only that the remainder is $\mathcal{O}(\lambda^3)$. Hence it is sufficient to check that there is at most one solution; this will be true if we prove it for a non–positive V and $\lambda > 0$. Then V_{00} is also non–positive, and excluding the trivial case $V=0$ we see that there is a positive C_1 such that $|z^{-1}| \le C_1\lambda^{-1}$ for small λ and any solution z of the equation (19). The operator–valued function $z \mapsto P_{\alpha(z)}$ is real–analytic for $z>0$ and has a bounded limit as $z \to 0+$, hence Cauchy integral formula gives

$$\left\|\frac{dP_{\alpha(z)}}{dz}\right\| < C_2|z^{-1}|$$

for some C_2 and small $|z|$. An explicit calculation shows that

$$\left(e^{-z|\cdot|}|V|^{1/2}\chi_0,\, \left[2|\cdot| + \frac{dP_{\alpha(z)}}{dz}\right] e^{-z|\cdot|}|V|^{1/2}\chi_0\right)$$

remains bounded as $z \to 0+$ since $V_{00} \in L^2(I\!R, |x|dx)$ by assumption. Then $\left|\frac{\partial G}{\partial z}\right|$ can be estimated by the sum of two terms; the one containing $\frac{dP_{\alpha(z)}}{dz}$ can be handled as in the Schrödinger–operator case [Si] being therefore $\le C_3\lambda$ for some C_3. On the other hand, the operator B_z of multiplication by $xe^{-z|x|}$ fulfils $\|B_z\| \le e^{-1}|z|^{-1}$ and the same argument applies; hence there is $C_4 > 0$ such that

$$\left|\frac{\partial G}{\partial z}\right| \le C_4\lambda$$

holds for $|z^{-1}| \le C_1\lambda^{-1}$ and all sufficiently small λ. Any two solutions $z_1,\, z_2$ of (19) have to fulfil

$$z_2 - z_1 = \int_{z_1}^{z_2} \frac{\partial G}{\partial z}\, dz$$

so the uniqueness is ensured for $\lambda < C_4^{-1}$.

It remains to prove that the term of order λ^2 is positive if $\int_{I\!R} \lambda V_{00}(x)\, dx = 0$ so the bound state exists also in this case. The corresponding Taylor coefficient is proportional to

$$\lim_{\varepsilon\to 0+} 2\int_{I\!R^2} V_{00}(x)\, \frac{e^{-\varepsilon|x-x'|}-1}{2\varepsilon}\, V_{00}(x')\, dx\, dx'$$

$$+ \sum_{N=1}^{\infty}\sum_{j=1}^{d_N} \int_{I\!R^2} V_{0N_j}(x)\, \frac{e^{-\sqrt{\kappa_N^2-\kappa_0^2}|x-x'|}}{\sqrt{\kappa_N^2-\kappa_0^2}}\, V_{N_j0}(x')\, dx\, dx'$$

$$= \lim_{\varepsilon\to 0+} 2\int_{I\!R} |\hat V_{00}(k)|^2 \frac{dk}{k^2+\varepsilon^2} + \sum_{N=1}^{\infty}\sum_{j=1}^{d_N} \int_{I\!R} |\hat V_{0N_j}(k)|^2 \frac{dk}{k^2+\kappa_N^2-\kappa_0^2} > 0\,.$$

4.2 Proof of Theorem 4.1

Consider first the two–dimensional case. We use the bounds (7), where

$$H_\pm := -(1\mp a\beta\|\gamma\|_\infty)^{-2}\partial_s^2 - \partial_u^2 + V_\beta(s,u)\,,$$

where V_β is the potential (3) referring to γ_β. By Theorem 4.2 each of the operators $H_\pm$ has for small β just one eigenvalue $e_\pm(\beta)$; the minimax principle tells us then that the same is true for H and $e_+(\beta) \ge e(\beta) \ge e_-(\beta)$.

Theorem 4.2 gives us an expansion of $e_\pm(\beta)$; if we rescale the longitudinal variable to $s_\pm := (1\mp a\beta\|\gamma\|_\infty)s$ and change appropriately the integration variables, we obtain

$$\sqrt{\kappa_1^2 - e_\pm(\beta)^2} \;=\; -\,\frac{1}{2}\,(1\mp a\beta\|\gamma\|_\infty)^{-1}\,\int_{I\!\!R} (V_\beta)_{11}(s)\,ds$$

$$-\,\frac{1}{4}\,(1\mp a\beta\|\gamma\|_\infty)^{-3}\left\{\int_{I\!\!R^2} (V_\beta)_{11}(s)|s-s'|(V_\beta)_{11}(s')\,ds\,ds'\right.$$

$$\left.-\,\sum_{N=2}^{\infty}\int_{I\!\!R^2} (V_\beta)_{1N}(s)\,\frac{e^{-\sqrt{\kappa_N^2-\kappa_1^2}|s-s'|}}{\sqrt{\kappa_N^2-\kappa_1^2}}\,(V_\beta)_{N1}(s')\,ds\,ds'\right\}$$

$$+\,\mathcal{O}(\beta^3)\,.$$

Since V_β itself expands in terms of β, we may neglect the scaling factors $1\mp a\beta\|\gamma\|_\infty$ when computing the leading term.

Let us write the right side as $I_1+\sum_{N=1}^{\infty} I_{2,N}+\cdots$. The first term is through an easy integration by parts equal to

$$I_1 \;:=\; \frac{\beta^2}{8}\int_{-a}^{a} du\int_{I\!\!R} ds\,\chi_1(u)^2\left[\frac{\gamma^2}{(1+u\beta\gamma)^2}\;-\;\frac{u^2\dot\gamma^2}{(1+u\beta\gamma)^4}\right]$$

$$=\;\frac{\beta^2}{8}\,\left\{\|\gamma\|^2-\;\|u\chi_1\|^2\|\dot\gamma\|^2\right\}\,+\,\mathcal{O}(\beta^3)\,;$$

we have used the fact that $\dot\gamma(s)\to 0$ as $|s|\to\infty$ due to *(d2)*. What is important is that the integration by parts cancels the term linear in β. Hence we have to compute $\sum_{N=1}^{\infty} I_{2,N}$ because it contains also contributions of order β^2 coming from the second term in (3). We have

$$I_{2,1} \;=\; -\,\frac{1}{4}\int_{I\!\!R^2} ds\,ds'\int_{-a}^{a}\int_{-a}^{a} du\,du'\chi_1(u)^2\chi_1(u')^2\,V_\beta(s,u)\,|s-s'|\,V_\beta(s')$$

$$=\;-\,\frac{\beta^2}{16}\int_{-a}^{a}\int_{-a}^{a} du\,du'\,uu'\,\chi_1(u)^2\chi_1(u')^2\int_{I\!\!R^2} ds\,ds'\,\ddot\gamma(s)\,|s-s'|\,\ddot\gamma(s')\,+\,\mathcal{O}(\beta^3)\,.$$

By a double integration by parts, the inner integral equals $-2\int_{I\!\!R}\dot\gamma(s)^2 ds$, so

$$I_{2,1}\;=\;\frac{\beta^2}{8}\,(\chi_1,u\chi_1)^2\|\dot\gamma\|^2+\,\mathcal{O}(\beta^3)\,.$$

The leading part in the remaining terms is

$$I_{2,N} \;=\; \frac{\beta^2}{16}\int_{-a}^{a}\int_{-a}^{a} du\,du'\,uu'\,\chi_1(u)\chi_N(u)\chi_1(u')\chi_N(u')$$

$$\times\;\int_{I\!\!R^2} ds\,ds'\,\ddot\gamma(s)\,\frac{e^{-\varrho_N|s-s'|}}{\varrho_N}\,\ddot\gamma(s')\,+\,\mathcal{O}(\beta^3)\,,$$

where the inner integral can be by a repeated integration by parts rewritten as

$$2\int_{I\!\!R}\dot\gamma(s)^2 ds\,+\,\varrho_N\int_{I\!\!R^2} ds\,ds'\,\dot\gamma(s)\,e^{-\varrho_N|s-s'|}\,\dot\gamma(s')\,.$$

Putting all the contributions together and using the Parseval identity, $\|u\chi_1\|^2 = \sum_{N=1}^{\infty}(\chi_N, u\chi_1)^2$, we find that the terms containing $\|\dot\gamma\|^2$ cancel and we arrive at the relation (14).

The proof for the three–dimensional case is completely analogous. The transverse eigenfunctions are now numbered conventionall starting from $N = 0$, and one has to replace $1+u\beta\gamma$ by $h^\beta := 1 + r\gamma_\beta\cos(\theta-\alpha)$, *i.e.*, $u\dot\gamma$, $u\ddot\gamma$ by h_s, h_{ss}, respectively. If the torsion is non–zero, of course, one cannot in general separate the integrations completely, and the Parseval identity in the last step has to be applied to the function $(s,r,\theta) \mapsto \chi_0(r,\theta)h_s(s,r,\theta)$ of $L^2(I\!R\times B_a)$. ∎

4.3 Remark. Mimicking the argument from the last part of the proof of Theorem 4.2, we check easily that the terms on the right sides of (14), (15) which express the contribution of higher transverse modes are positive. They are small in thin tubes when the exponential kernel is decaying fast. In fact, we have the estimate

$$\begin{aligned}\sum_{N=2}^{\infty} I_{2,N} &= \frac{\beta^2}{8}\sum_{N=2}^{\infty}\varrho_N^2\,(\chi_n, u\chi_1)^2\int_{I\!R}|\hat{\dot\gamma}(k)|^2\frac{dk}{k^2+\varrho_N^2}\\ &\le \frac{\beta^2}{8}\sum_{N=1}^{\infty}(\chi_n, u\chi_1)^2\,\|\hat{\dot\gamma}\|^2 = \frac{\beta^2}{8}\|\dot\gamma\|^2\,\|u\chi_1\|^2\end{aligned}$$

in two dimensions, and similarly

$$\sum_{N=1}^{\infty} I_{2,N} \le \frac{\beta^2}{8}\|\chi_0 h_s\|^2$$

for a three–dimensional tube, so these terms are of order $\mathcal{O}(a^2)$ as $a\to 0$.

5 Perturbation theory: thin tubes

Now we are going to return to the situation where the tube axis is any curve which satisfies our assumptions about regularity and decay of the curvature, and to study the behaviour of the bound state eigenvalues in the limit $a\to 0$.

We shall treat the two– and three–dimensional cases on the same footing; the corresponding Schrödinger operator is denoted as $-\partial_s b\partial_s - \Delta_{B_a} + V$ acting on $L^2(I\!R, ds)\otimes L^2(B_a, du)$ where B_a is the ball of radius a in the transverse variable u in $I\!R$ or $I\!R^2$, respectively, according to the dimension, and $du := r\,dr\,d\theta$ in the latter case. The functions b and V are defined by (2) and (3) for the two–dimensional case and by (11) and (12) for dimension three. We adopt the following conventions to unify the notations between the two cases:

$$h(s,u) := h(s,r,\theta) := 1 + r\,\gamma(s)\,\cos(\theta-\alpha(s))\,,$$

$$b \;:=\; h^{-2}, \quad V \;:=\; -\frac{\gamma^2}{4h^2} + \frac{1}{2}\frac{h_{ss}}{h^3} - \frac{5}{4}\frac{h_s^2}{h^4}\,, \tag{21}$$

where $u = \left(r,\, \frac{\pi}{2} \mp \frac{\pi}{2}\right)$ and $\tau = \alpha = 0$ in the two–dimensional situation. It is convenient to replace the Hamiltonian by the following unitarily equivalent operator acting on $L^2(I\!R \times B_1)$:

$$H \;:=\; -a^{-2}\Delta_{B_1} + T\,, \quad T \;:=\; T(a) \;:=\; -\partial_s b(s,au)\partial_s + V(s,au)\,, \tag{22}$$

which is obtained by the scaling $(s,u) \to (s,au)$; we shall also denote by b and V the functions $(s,u) \mapsto b(s,au)$ and $(s,u) \mapsto V(s,au)$, respectively.

As in the previous chapter, an important ingredient here is the transverse–mode decomposition. If χ_j denotes the j–th eigenfunction of $-\Delta_{B_1}$ with eigenvalue E_j, we introduce the embedding $J_j \,:\, L^2(I\!R, ds) \to L^2(I\!R, ds) \otimes \{\chi_j\} \subset \mathcal{H}$ and its adjoint J_j^* ; the latter can be regarded as the projection onto the j–th mode χ_j of $-\Delta_{B_1}$. This allows us to express H as an infinite matrix differential operator, $(H_{j,k})_{j,k=1}^{\infty}$ with

$$H_{j,k} := J_i^* H J_k \;=\; a^{-2}E_j\delta_{j,k} + T_{j,k}\,, \quad T_{j,k} \;:=\; -\partial_s b_{j,k}\partial_s + V_{j,k}\,, \tag{23}$$

where $b_{j,k} := \int_{B_1} b(\cdot,au)\,\overline{\chi}_j(u)\chi_k(u)\,du$ and $V_{j,k} := \int_{B_1} V(\cdot,au)\,\overline{\chi}_j(u)\chi_k(u)\,du$; we set $H_j := H_{j,j}$, $T_j := T_{j,j}$ *etc.* In the most part of the following analysis, we shall consider the simplest comparison operator

$$H^0 \;:=\; -a^{-2}\Delta_{B_1} + T^0 \otimes I\,, \quad T^0 \;:=\; -\partial_s^2 + V^0 \;:=\; -\partial_s^2 - \frac{1}{4}\gamma^2\,. \tag{24}$$

Suppose that γ is such that $\sigma_{ess}(T^0) = I\!R_+$ and $\sigma_d(T^0) \neq \emptyset$, and let λ be one of the negative eigenvalues of T^0. Obviously, $E^0 := a^{-2}E_1 + \lambda$ is then a discrete eigenvalue of H^0 ; we want to show that it gives rise to an eigenvalue of H for a small enough a when the perturbation $H - H^0$ is turned on, and to derive the corresponding perturbation expansion.

5.1 The main theorem

To state the main result of this chapter, we introduce the following notation for the perturbation:

$$\begin{aligned} W \;&:=\; H - H^0 \;=\; -\partial_s(b(s,au)-1)\partial_s + V(s,au) + \frac{1}{4}\gamma(s)^2\,, \\ W_{j,k} \;&:=\; J_j^* W J_k \;=\; -\partial_s(b_{j,k} - \delta_{j,k})\partial_s + V_{j,k} + \frac{1}{4}\gamma^2\delta_{j,k}\,. \end{aligned} \tag{25}$$

We shall also use the formal expansion of the function $W_{j,k}$ into power series in a,

$$W_{j,k} \;=\; \sum_{l=1}^{\infty} W_{j,k}^{(l)}\,a^l \tag{26}$$

which is actually convergent in the topology of $\mathcal{B}(\mathcal{H}^2(I\!R), L^2(I\!R))$ for all a small enough (see Lemma 5.2 below). Notice that $W_{j,k}$ as well as $W_{j,k}^{(l)}$ are second order differential operators in the variable s exclusively, in particular,

$$W_{j,k}^{(l)} = -\partial_s b_{j,k}^{(l)} \partial_s + V_{j,k}^{(l)} \tag{27}$$

with

$$b_{j,k}^{(l)} := (l+1)\,\gamma^l \int_{B_1} (-r\cos(\theta-\alpha))^l\, \overline{\chi}_j(u)\chi_k(u)\,du$$

and

$$\begin{aligned} V_{j,k}^{(l)} :=\; & \frac{1}{4}(l+1)\,(-\gamma)^{l-2} \int_{B_1} (r\cos(\theta-\alpha))^{l-2} r^2 \\ & \times \Big\{ \left[-\gamma^4 - l\gamma(\ddot{\gamma}-\gamma\tau^2)\right] \cos^2(\theta-\alpha) \\ & - \left[l\gamma(2\dot{\gamma}\tau+\gamma\dot{\tau}) + \frac{5}{3}\,l(l-1)\gamma\dot{\gamma}\tau \right] \sin(\theta-\alpha)\cos(\theta-\alpha) \\ & - \frac{5}{6}\,l(l-1)\gamma^2\tau^2 \sin^2(\theta-\alpha) \Big\}\, \overline{\chi}_j(u)\chi_k(u)\,du\,; \end{aligned}$$

recall that with our convention $\int_{B_1} f(s,r,\theta)\,du = \int_{B_1} f(s,r,\theta)\,r\,dr\,d\theta$ for the three–dimensional waveguide and

$$\int_{B_1} f(s,r,\theta)\,du = \int_0^1 f(s,r,0)\;du + \int_{-1}^0 f(s,r,\pi)\;du$$

in dimension two. Now we are ready to state the main result of this chapter.

5.1 Theorem. *Assume (r1–4) and (d1), then*

(a) each discrete eigenvalue λ of T^0 gives rise for a small enough to an eigenvalue E of H of multiplicity one, which is given by an absolutely convergent series,

$$E = a^{-2}E_1 + \lambda + \sum_{m=1}^{\infty} e_m\,,$$

where the coefficients e_m are of order $\mathcal{O}(a^m)$ as a goes to zero; the expressions for them are given by (29) below;

(b) conversely, for any discrete eigenvalue E of H there is a unique discrete eigenvalue λ of T^0 such that

$$E - a^{-2}E_1 - \lambda = \mathcal{O}(a)\,;$$

(c) each coefficient e_m is a C^∞ function of the variable a in the interval $[0,a_0)$ for some positive a_0,

(d) the coefficient e_1 *is analytic in* a *around* $a=0$ *and can be expressed as*

$$e_1 = \sum_{l=1}^{\infty} e_{1,l}\, a^l\,, \qquad e_{1,l} := (\varphi, W_1^{(l)}\varphi)\,,$$

where φ *is the eigenvector of* T^0 *associated with* λ *; recall that* $W_1^{(l)} := W_{1,1}^{(l)}$ *.*

5.2 Proof of Theorem 5.1

We begin with the analyticity properties of W in the variable a.

5.2 Lemma. *The operators* W *form a type* A *analytic family of self–adjoint operators with respect to* a *around* $a=0$ *; its domain is* $\mathcal{H}^2(\mathbb{R})\otimes L^2(B_1)$ *.*

Proof. Since b and V are analytic in r around the point $r=0$, the same is true for $a\mapsto b(s,au)$ and $a\mapsto V(s,au)$ regarded as operator–valued functions of the variable a; in addition, $b(s,au)$ is strictly positive for all s and u, and any a small enough. Hence T, and therefore also $W=T-T(0)$ is a type A analytic family [Ka, Chap.VII] with the domain $\mathcal{H}^2(\mathbb{R})\otimes L^2(B_1)$ for small a. ∎

In view of the assumptions we know that $\sigma_{ess}(T^0)=\mathbb{R}_+$, the operator T^0 has at least one discrete eigenvalue and all its discrete eigenvalues are simple (see, *e.g.*, [BGS]). Taking further into account that the spectrum of T^0 is bounded from below by $-\frac{1}{4}\|\gamma\|_\infty^2$, we see that the discrete spectrum of H^0 is non–empty and simple for a small enough.

Following the standard perturbation–theory procedure, we shall consider a contour Γ enclosing a single eigenvalue $E^0=a^{-2}E_1+\lambda$ and show that the perturbation W is uniformly small on Γ. To be more specific, we choose Γ so that $\Gamma-a^{-2}E_1$ is a circle centered at λ in the resolvent set of T^0. Let a_1 be the radius of the circle in which W is analytic; furthermore, we denote by R^0, R the resolvents of H^0, H, respectively, and by $\hat{R}^0$ the reduced resolvent with respect to E^0.

5.3 Lemma. *There are constants* $c^{(1)}$, $c_\Gamma^{(2)}$ *such that for all* $a<a_1$ *one has*

(a) $\|W(-\partial_s^2+1)^{-1}\|\le c^{(1)}a$,

(b) $\|WR^0(z)\|\le c_\Gamma^{(2)}a$ *for all* $z\in\Gamma$,

(c) $\|W\hat{R}^0(E^0)\|\le c_\Gamma^{(2)}a$.

Proof. By a straightforward computation (see also [DEŠ2]) one readily shows that

$$|W|^2 \le 4\|b-1\|^2\partial_s^4 - 4\|\dot{b}\|^2\partial_s^2 + 2\|V-V^0\|^2$$

holds in the form sense on $\mathcal{H}^2(I\!R) \otimes L^2(B_1)$; this implies the assertion (a) since $b-1$, $\dot{b}$ and $V-V^0$ are obviously $\mathcal{O}(a)$ uniformly in s and u as a goes to zero.

To check the second assertion we write $WR^0(z) = W(-\partial_s^2+1)^{-1}(-\partial_s^2+1)R^0(z)$ for a fixed $z_0 \in \Gamma$. In view of (a), it is sufficient to show that $(-\partial_s^2+1)R^0(z)$ is $\mathcal{O}(1)$ on Γ as a goes to zero; this follows easily, *e.g.*, using the transverse mode decomposition of $R^0(z)$ — see [DEŠ2]. Finally, the same argument applies to the reduced resolvent $\hat{R}^0(E^0)$ giving (c). ∎

By the part (b) of the above lemma, the contour Γ lies also in the resolvent set of H for a small enough; we may therefore define the corresponding spectral projection P and compare it to P^0, the one of H^0:

$$P - P^0 \;=\; \frac{i}{2\pi}\int_\Gamma R^0(z)WR^0(z)(1+WR^0(z))^{-1}\,dz\,.$$

The difference $P-P^0$ is $\mathcal{O}(a)$ since $WR^0(z)$ is $\mathcal{O}(a)$ and $R^0(z)$ is $\mathcal{O}(1)$ as a goes to zero. Thus P and P^0 have the same dimension for a small enough which shows that H has inside Γ a single eigenvalue E, and that E is simple. The eigenvalue shift $E-E^0$ can be computed perturbatively following [Ka, Sec.2.2]:

$$E - E^0 \;=\; \sum_{m=1}^{\infty} e_m\,, \qquad e_m \;:=\; \frac{i}{2\pi}\,\mathrm{tr}\int_\Gamma (z-E^0)R^0(z)(-WR^0(z))^m\,dz\,. \tag{28}$$

Evaluating the contour integral we obtain

$$e_m \;=\; \frac{(-1)^m}{m}\sum_{p_1+\cdots+p_m=m-1}\mathrm{tr}\prod_{i=1}^{m} WS^{(p_i)}\,, \tag{29}$$

where $S^{(p_i)}$ denotes $-P^0$ if $p_i=0$ and $\hat{R}^0(E^0)^{p_i}$ otherwise. Each term of the product on the *rhs* of (29) contains at least one one–dimensional projection, so the trace can be estimated by the norm; we have

$$\|WP^0\| \;\le\; \frac{1}{2\pi}\int_\Gamma \|WR^0(z)\|\,dz \;\le\; \frac{|\Gamma|}{2\pi}\,c_\Gamma^{(2)}a\,,$$

$$\|W\hat{R}^0(E^0)^{p_i}\| \;\le\; c^{(1)}c_\Gamma^{(2)}a$$

for $p_i=0$ and $p_i\neq 0$, respectively. Since there are at most m–1 projections among the operators S^{p_i} we get

$$\left\|\prod_{i=1}^{m} WS^{(p_i)}\right\| \;\le\; \left(c^{(1)}\right)^m\left(\tilde{c}_\Gamma^{(2)}\right)^{2m-2}\,a^m\,,$$

where we have set $\tilde{c}_\Gamma^{(2)} := \max\left\{1,\,c_\Gamma^{(2)},\,\frac{|\Gamma|}{2\pi}\,c_\Gamma^{(2)}\right\}$. Finally, the number of terms at the *rhs* of (29) is $\left(\begin{smallmatrix}2m-2\\ m-1\end{smallmatrix}\right)$ so we obtain

$$|e_m| \;\le\; \left(\sqrt{c^{(1)}}\,\tilde{c}_\Gamma^{(2)}\right)^{2m}\left(\begin{array}{c}2m-2\\ m-1\end{array}\right)\frac{a^m}{m}\,. \tag{30}$$

The *rhs* is easily seen to define a convergent series; this concludes the proof of the assertion (a) of Theorem 5.1.

The part (b) follows from the generalized "convergence" of H to H^0 as $a \to 0$ in the sense of Kato which means that $(H-z)^{-1}-(H^0-z)^{-1}$ converges to zero in the norm for a fixed z that belongs to both the resolvent sets of H and H^0 ; this is an obvious consequence of Lemma 5.3. We use the quotation marks because H^0 is in fact a–dependent, however, it can be seen easily that the argument of [Ka] goes through in this case.

To prove the assertion (c) we use the formula (29). We set $a_0 := \min\{1, 1/c_\Gamma^{(2)}\}$ and notice that WP^0 is bounded analytic around $a=0$ due to Lemma 5.2 and the fact that P^0 is a–independent. Thus it remains to check that $W\hat{R}^0(E^0)^{p_i}$ is bounded and C^∞ on $[0,a_0)$ since the smoothness properties are preserved when the trace with a constant projection P^0 is taken.

5.4 Lemma. *The reduced resolvent as a function of a satisfies the conditions*

(a) $\hat{R}^0(E^0) \in C^\infty([0,a_0),\, \mathcal{B}(\mathcal{H}))$,

(b) $\hat{R}^0(E^0)\Big|_{a=0} = \left((T^0-\lambda)^{-1}\right)^{\hat{}} \oplus 0$,

(c) $\left(\frac{d}{da}\right)^m \hat{R}^0(E^0)\Big|_{a=0} = 0$ *for any positive integer* m .

Proof. The transverse–mode decomposition yields the relation

$$\hat{R}^0(E^0) \;=\; \left((T^0-\lambda)^{-1}\right)^{\hat{}} \;\oplus\; \bigoplus_{k=2}^{\infty} (T^0 + a^{-2}(E_k - E_1) - \lambda)^{-1} \tag{31}$$

from which we readily deduce that the norm limit of $\hat{R}^0(E^0)$ as a goes to zero gives the assertion (b). To prove the rest we observe that $\hat{R}^0(E^0)$ is in fact bounded analytic in $(0,a_0)$ and its derivative equals

$$\frac{d}{da}\,\hat{R}^0(E^0) \;=\; 0 \oplus \bigoplus_{k=2}^{\infty} (T^0 + a^{-2}(E_k-E_1) - \lambda)^{-2} 2a^{-3}(E_k-E_1)\;;$$

hence it is bound from above by $2a(E_2-E_1)^{-1}$. It follows that $\hat{R}^0(E^0)$ is actually C^1 at $a=0$ and has zero derivative there. Since this argument can be repeated for all successive derivatives, the assertion (a) and (c) are proven ∎

In this way, we have checked (c). Finally the assertion (d) is obvious because $e_1 = \mathrm{tr}\,(WP^0)$, the operator–valued function W is analytic in a around $a=0$ and P^0 is a–independent.

5.3 Remarks

After finishing the proof, let us make a few comments. Notice first that under the assumptions of the theorem, all the coefficients e_m as functions of a are C^∞ at $a = 0$. Since $e_m = \mathcal{O}(a^m)$ as a goes to zero we see that *all eigenvalues of H admit an asymptotic expansion in a up to any prescribed order.* This result requires no smoothness conditions on the reference curve Γ other than those expressed by *(r1)*.

The next item to mention is the *contribution of mode–coupling terms.* A close look at the coefficients e_2 and e_3 shows that these terms in the perturbation W contribute only to the $\mathcal{O}(a^4)$ order. Indeed, one has

$$e_2 \;=\; -\operatorname{tr}\left(P^0 W \hat{R}^0(E^0) W P^0\right) \;=\; \sum_{k=1}^{\infty} e_2^k$$

with

$$e_2^1 \;:=\; -\left(W_1\varphi, \left((T^0 - \lambda)^{-1}\right)\hat{}\; W_1\varphi\right)$$

and

$$e_2^k \;:=\; -\left(W_{k,1}\varphi, (T^0 + a^{-2}(E_k - E_1) - \lambda)^{-1} W_{k,1}\varphi\right) \quad \text{if} \quad k \geq 2\,.$$

It is clear that all e_2^k, $k \geq 2$, contain the "off–diagonal" part of W coupling the first mode to the higher ones, and therefore they are $\mathcal{O}(a^4)$, whereas e_2^1 may contain terms of order two or three because

$$e_2^1 \;=\; \sum_{l=2}^{\infty} e_{2,l}^1\, a^l\,,$$

where

$$e_{2,l}^1 \;:=\; -\sum_{m=1}^{l-1} \left(W_1^{(l-m)}\varphi, \left((T^0 - \lambda)^{-1}\right)\hat{}\; W_1^{(l)}\varphi\right), \qquad l \geq 2\,.$$

A similar calculus leads to the same conclusion for e_3. Thus we may infer that the mode–coupling terms of W begin to contribute to the perturbation expansion of the eigenvalues only at the order four. An alternative view on this property is provided by the so–called adiabatic approximation.

5.4 The adiabatic operator

If we discard the off–diagonal terms in (23) we get another approximation of H suitable for comparison, namely

$$H^1 \;:=\; \bigoplus_{j=1}^{\infty} \left(a^{-2}E_j + T_j\right),$$

which we shall call the *adiabatic operator*. Since it contains the weight factor in the kinetic part, it is naturally expected to approximate H more closely than H^0 ; we want to show in conclusion of this chapter that this is indeed the case. The operators T_j are, of course, a–dependent but they approach T^0 as $a \to 0$.

5.5 Lemma. *T_j converges to T^0 for each $j \geq 1$ in the norm resolvent sense when a goes to zero.*

Proof. This is obviously true because T_j is analytic in a and $T_j|_{a=0} = T^0$. ∎

It follows that for small enough a, the operator T_1 has a discrete spectrum below zero, each eigenvalue having multiplicity one; any of these eigenvalues converges to one of T^0, and conversely, each eigenvalue of T^0 is the limit of an eigenvalue of T_1 as a goes to zero.

5.6 Theorem. *Assume (r1–4) and (d1), then there is a bijective correspondence between the discrete spectrum of H and that of T^1 in the following sense:*

(a) each discrete eigenvalue of H^1 of the form $E^1 = a^{-2}E_1 + \lambda^1$, where λ^1 is a discrete eigenvalue of T^1 (depending on a), gives rise to an eigenvalue E of H for all a small enough;

(b) conversely, for any discrete eigenvalue E of H there is a unique discrete eigenvalue λ^1 of T^1 such that

$$\lim_{a\to\infty} (E - a^{-2}E_1 - \lambda^1) \,=\, 0\,.$$

Moreover, $E - a^{-2}E_1 - \lambda^1 = \mathcal{O}(a^4)$ holds as a goes to zero.

Proof. The argument is similar to the one used above, so we limit ourselves to a sketch. Let $\tilde{W} := H - H^1$. Mimicking the proof of Lemma 5.3 one can show that $\tilde{W}(H^1 - z)^{-1} = \mathcal{O}(a)$ as $a \to 0$ uniformly in z belonging to a contour Γ around $a^{-2}E_1 + \lambda$, where $\lambda := \lim_{a\to 0}\lambda^1$ is a discrete eigenvalue of T^0. This implies, in particular, that $(H-z)^{-1} - (H^1-z)^{-1}$ converges to zero in norm for $a \to 0$, and therefore the discrete spectrum of H^1 is stable (in the sense of [Ka]) under the perturbation $\tilde{W}$, and moreover, that the bijective correspondence stated in the theorem is valid. To estimate $E-E^1$, we use then the well–known formula

$$E - E^1 \,=\, -\,\mathrm{tr}\,\left(P^1\tilde{W}Q^1(Q^1(H-E)Q^1)^{-1}Q^1\tilde{W}P^1\right)\,,$$

where P^1 is the eigenprojection of H^1 associated to E^1 and $Q^1 := I - P^1$. Since $P^1\tilde{W}Q^1 = \mathcal{O}(a)$ and $(Q^1(H-E)Q^1)^{-1} = \mathcal{O}(a^2)$ we arrive at the last assertion of the theorem. ∎

6 Some open problems

In conclusion, let us mention some directions in which the above mentioned results can be strengthened or extended. The list of problems we present below is by far not exhaustive, other interesting open questions can be found, *e.g.*, in [EŠ4].

As usually in a mathematical theory, one wants to ask whether the used assumptions can be replaced by weaker ones. The regularity requirements in Theorems 2.1 and 3.3 seem to be to be optimal, at least within the "straightening" approach, while the sufficient conditions in the subsequent corollaries allow various modifications. It is also desirable to extend the results to tubes with a non–smooth boundary and locally changing cross section, where the existence of the bound states have been demonstrated up to now in several examples only.

Other obvious generalizations are tubes in $I\!\!R^n$, $n>3$, a curved Dirichlet layer in $I\!\!R^n$ and similar structures. No rigorous result of that type is known to us though some formal calculations have been made [dC1, dC2, To]. The first named case seems to be of a rather mathematical interest while the other provides, in addition, for $n=3$ a rough model of a thin semiconductor film as discussed in the introduction. The problem is, however, more complicated now; the mentioned formal results suggest that the leading term in the effective potential analogous to (3) and (12) can be zero in a curved part of the layer if the generating surface is locally spherical.

As mentioned in Section 2.3, a thin curved strip supports typically one bound state if the curvature has one well distinguished peak. If there are more clearly separated bends one conjectures that a bound state is associated with each of them and the wavefunctions are localized in the vicinity of the bends. One may attempt to estimate the shift of the eigenvalues comparing to corresponding one–bend tubes in analogy with the tunneling analysis of multiwell Schrödinger operators [BCD], [CDS, HeSj, Hel].

An entirely new class of effects opens when we replace the assumptions about the decay of curvature by a periodicity hypothesis. In this case one expects that a thin tube would have a band–type spectrum but it remains to be proven. Further extensions include quasiperiodically curved tubes, tubes with a random curvature *etc.* However, the continuous spectrum is important also for the tubes considered here — as a part of the scattering analysis.

The effective attractive potential responsible for existence of the bound states generates at the same time resonances below the thresholds of the higher transversal modes as can be shown for a two–dimensional curved strip by combination of complex scaling and perturbation techniques [DEŠ1, DEŠ2]. In these papers also the Fermi–rule contribution to the resonance width was computed and shown to be exponentially small in the limit $d\to 0$. One can conjecture that the same is true for the full resonance width and that this result extends to curved three-dimensional tubes.

Acknowledgments

Most of the results reviewed here was obtained during the visits of P.D. to the Laboratory of Theoretical Physics, JINR Dubna and Nuclear Physics Institute AS CR, Řež, and P.E. to the Université de Toulon et du Var and C.P.T. C.N.R.S., Marseille; the authors express their gratitude to the hosts. The work was partially supported by the AS CR Grant No.148409.

References

[AS] M.Abramowitz, I.Stegun: *Handbook of Mathematical Functions*, National Bureau of Standards, Washington 1964.

[AE] M.S.Ashbaugh, P.Exner: Lower bounds to bound state energies in bent tubes, *Phys.Lett.*__A150__ (1990), 183-186.

[ABGM] Y.Avishai, D.Bessis, B.M.Giraud, G.Mantica: Quantum bound states in open geometries, *Phys.Rev.* **B44** (1991), 8028–8034.

[Ba] H.U.Baranger: Multiprobe electron waveguides: Filtering and bend resistances, *Phys.Rev.* **B42** (1990), 11479–11495.

[BGS] R.Blanckenbecler, M.L.Goldberger, B.Simon: The bound states of weakly coupled long-range on-dimensional quantum Hamiltonians, *Ann.Phys.* **108** (1977), 89-78.

[BCD] P.Briet, J.–M.Combes, P.Duclos: Spectral stability under tunneling, *Commun.Math.Phys.* **126** (1989), 133–156.

[BLD] J.D.Bishop, J.C.Licini, G.J.Dolan: Lithium quench–condensed microstrucures and the Aharonov–Bohm effect, *Appl.Phys.Lett* **46** (1985), 1000-1002.

[CJ] J.J.Cambell, W.R.Jones: Symetrically truncated right–angle corners in parralel–plate and rectangular waveguides, *IEEE Transactions: MTT* **16** (1974), 687–696.

[CLM1] J.P.Carini, J.T.Londergan, K.Mullen, D.P.Murdock: Bound states and resonances in quantum wires, *Phys.Rev.* **B46** (1992), 15538–15541.

[CLM2] J.P.Carini, J.T.Londergan, K.Mullen, D.P.Murdock: Multiple bound states in sharply bent waveguides, *Phys.Rev.* **B48** (1993), 4503–4514.

[CDS] J.-M.Combes, P.Duclos, R.Seiler: Krein's formula and one–dimensional multiple well, *J.Funct.Anal.* **52** (1983), 257–301.

[dC1] R.C.T.da Costa: Quantum mechanics of a constrained particle, *Phys.Rev.* **A23** (1981), 1982-1987.

[dC2] R.C.T.da Costa: Constraints in quantum mechanics, *Phys.Rev.* **A25** (1982), 2893–2900.

[dC3] R.C.T.da Costa: Constrained particles in quantum mechanics, *Lett.N. Cim.* **36** (1983), 393–396.

[DB] S.Datta, S.Bandyopadhyay: Aharonov–Bohm effect in semiconductor microstructures, *Phys.Rev.Lett.* **58** (1987), 717–720.

[DMB] S.Datta, M.R.Melloch, S.Bandyopadhyay: Novel interference effect between parallel quantum wells, *Phys.Rev.Lett.* **55** (1985), 2344–2347.

[DE] P.Duclos, P.Exner: Curvature *vs.* thickness in quantum waveguides, *Czech.J.Phys.* **41** (1991), 1009–1018; erratum **42** (1992), 344.

[DEŠ1] P.Duclos, P.Exner, P.Šťovíček: Resonances at bends of a two–dimensional quantum waveguide, in *Proceedings of the Conference "Stochastic Processes, Physics and Geometry" (Locarno 1991)*, World Scientific, to appear

[DEŠ2] P.Duclos, P.Exner, P.Šťovíček: Curvature–induced resonances in a two–dimensional Dirichlet tube, submitted to *Ann.Inst.H.Poincaré*

[DJ] G.Dunne, R.L.Jaffe: Bound states in twisted Aharonov–Bohm tubes, *Ann.Phys.* **223** (1993), 180–196.

[E1] P.Exner: A model of resonance scattering on curved quantum wires, *Ann.Physik* **47** (1990), 123-138.

[E2] P.Exner: Bound states and resonances in quantum wires, in *Order, Disorder and Chaos in Quantum Systems*, Birkhäuser, Basel 1990; pp.65-85.

[E3] P.Exner: Bound states in quantum waveguides of a slowly decaying curvature, *J.Math.Phys.* **34** (1993), 23–28.

[EŠ1] P.Exner, P.Šeba: Bound states in curved quantum waveguides, *J.Math. Phys.* **30** (1989), 2574-2580.

[EŠ2] P.Exner, P.Šeba: Trapping modes in a curved electromagnetic waveguide with perfectly conducting walls, *Phys.Lett.* **A144** (1990), 347-350.

[EŠ3] P.Exner, P.Šeba: A new type of quantum interference transistors, *Phys. Lett.* **A129** (1988), 477–480.

[EŠ4] P.Exner, P.Šeba: Electrons in semiconductor microstructures: a challenge to operator theorists, in *Schrödinger Operators, Standard and Non–Standard*, World Scientific, Singapore 1989; pp.85–106.

[EŠŠ1] P.Exner, P.Šeba, P.Šťovíček: On existence of a bound state in an L-shaped waveguide, *Czech.J.Phys.*~**B39** (1989), 1181-1191.

[EŠŠ2] P.Exner, P.Šeba, P.Šťovíček: Semiconductor edges can bind electrons, *Phys.Lett.*~**A150** (1990), 179-182.

[Go] Ch.Goldstein: Scattering theory in waveguides, in *Scattering Theory in Mathematical Physics*, D.Reidel, Dordrecht 1974; pp.35–51.

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

[HH] A.Harwitt, J.S.Harris: Observation of Stark shifts in quantum well intersubband transition, *Appl.Phys.Lett.* **50** (1987), 685–687.

[He] J.Hersch: Sur la frequence fondamentale d'une membrane vibrante: évalu- ations par defaut et principle de maximum, *ZAMP* **11** (1960), 387–413.

[Hel] B.Helffer: *Semi–Classical Analysis for the Schrödinger Operator and Applications*, Lecture Notes in Mathematics, vol.1336, Springer, Berlin 1988.

[HeSj] B.Helffer, J.Sjöstrand: Multiple wells in the semiclassical limit, *Commun. in PDE* **9** (1984), 337–408.

[IN] H.Ishio, K.Nakamura: Quantum transport in open billiards: dependence on the degree of opening, *J.Phys.Soc. Japan* **61** (1992), 2649–2654.

[JK] H.Jensen, H.Koppe: Quantum mechanics with constraints, *Ann.Phys.* **63** (1971), 586–591.

[Ka] T.Kato: *Perturbation Theory for Linear Operators*, Springer Verlag, Berlin 1966.

[KLR] A.A.Kirilenko, V.R.Litvinov, L.A.Rudj: Truncated bend of a rectangukar waveguide in the H–plane, *Sov.J.Radiotechnics and Electronics* **24** (1979), 1032–1052.

[KRS] A.A.Kirilenko, L.A.Rudj, V.P.Shestopalov: Wave scattering on a waveguide bend, *Sov.J.Radiotechnics and Electronics* **19** (1974), 687–696.

[KRT] A.A.Kirilenko, L.A.Rudj, V.I.Tkachenko: Diffraction on an E–plane of a rectangular waveguide, *Sov.J.Radiotechnics and Electronics* **30** (1985), 918–924.

[Kl] M.Klaus: On the bound state of Schrödinger operators in one dimension, *Ann.Phys.* **108** (1977), 288-300.

[KJ] H.Koppe, H.Jensen: Das Prinzip von d'Alembert in der klassischen Mechanik und in der Quantenmechanik, *Sitz.ber.Heidelberger Akad.Wiss.* (1971), 127–140.

[Marc] M.Marcuritz: *Waveguide handbook*, Dover, New York 1964.

[Ma] J.Marcus: On the analytical mechanics of chemical reactions. Quantum mechanics of linear collisions, *J.Chem.Phys.* **45** (1966), 4493–4499.

[Me] R.Mehran: Calculation of microstrip bends and Y–junstions with arbitrary angle, *IEEE Transactions: MTT* **26** (1978), 400–405.

[New] R.G.Newton: Bounds for the number of bound states for Schrödinger equation in one and two dimensions, *J.Operator Theory* **10** (1983), 119-125.

[NI] K.Nakamura, H.Ishio: Quantum transport in open billiards: comparison between circle and stadium, *J.Phys.Soc. Japan* **61** (1992), 3939–3944.

[Pi] D.Picca: Constraints in quantum mechanics, *Lett.N.Cim.* **36** (1982), 449–452.

[RS] M.Reed, B.Simon: *Methods of Modern Mathematical Physics, IV. Analysis of Operators*, Academic Press, New York 1978.

[Sa] H.Sakaki: Advances in microfabrication and microstructure physics, in *Foundations of Quantum Mechanics in the Light of New Technology*, Physical Society of Japan, Tokyo 1984; pp.94–110.

[SRW] R.L.Schult, D.G.Ravenhall, H.W.Wyld: Quantum bound states in a classically unbounded system of crossed wires, *Phys.Rev.* **B39** (1989), 5476–5479.

[Se] N.Seto: Bargmann's inequalities in spaces of arbitrary dimension, *Publ. RIMS* **9** (1974), 429–461.

[Si] B.Simon: The bound state of weakly coupled Schrödinger operators in one and two dimensions, *Ann.Phys.* **97** (1976), 279-288.

[SMRH] F.Sols, F.Macucci, U.Ravaioli, K.Hess: On the possibility of transistor action based on quantum interference phenomena, *Appl.Phys.Lett.* **54** (1989), 350–352.

[SRS] E.Switkes, E.L.Russell, J.L.Skinner: Kinetic energy and path curvature in bound state systems, *J.Chem.Phys.* **67** (1977), 3061–3067.

[TDP] H.Temkin, G.J.Dolan, M.B.Panish: Low–temperature photoluminiscence from InGaAs/InP quantum wires and boxes, *Appl.Phys.Lett.* **50** (1989), 2081–2084.

[TBV] G.Timp *et al.*: Propagation around a bend in a multichannel electron waveguide, *Phys.Rev.Lett.* **60** (1988), 2081-2084.

[To] 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.

[TG] C.Y.Tsao, W.A.Gambling: Curvilinear optical fibre waveguide: characterization of bound modes and radiative field, *Proc.Roy.Soc.London* **A425** (1989), 1–16.

[UHL] C.P.Umbach *et al.*: Direct observation of ensemble averaging of the Aharonov–Bohm effect in normal–metal loops, *Phys.Rev.Lett.* **56** (1986), 386–389.

[VOK1] K.Vacek, A.Okiji, H.Kasai: Multichannel ballistic magnetotransport
through quantum wires with double circular bends, *Phys.Rev.* **B47** (1993), 3695–3705.

[VOK2] K.Vacek, A.Okiji, H.Kasai: Ballistic transport in quantum wires with periodic bend structure, *Solid State Commun.* **85** (1993), 507–520.

[WWU] R.A.Webb *et al.*: The Aharonov–Bohm effect in normal metal — non–ensemble averaged quantum transport, *Physica* **A140** (1986), 175–182.

[WS] Hua Wu, D.L.Sprung: Multi–bend quantum wire, *Phys.Rev.* **B47** (1993), 1500–1506.

[WSM1] Hua Wu, D.L.Sprung, J.Martorell: Effective one–dimensional well for two–dimensional quantum wires, *Phys.Rev.* **B45** (1992), 11960–11967.

[WSM2] Hua Wu, D.L.Sprung, J.Martorell: A comparison of confining potentials in the quantum wire problem, *Appl.Phys.* **A56** (1993), 127–131.

[WSMK] Hua Wu, D.L.Sprung, J.Martorell, S.Klarsfeld: Quantum wire with periodic serial structure, *Phys.Rev.* **B44** (1991), 6351–6360.