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Generalised Quantum Waveguides

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Abstract. We study general quantum waveguides and establish explicit effective Hamiltonians for the Laplacian on these spaces. A conventional quantum waveguide is an ε-tubular neighbourhood of a curve in $\mathbb{R}^3$ and the object of interest is the Dirichlet Laplacian on this tube in the asymptotic limit $\varepsilon \ll 1$. We generalise this by considering fibre bundles M over a complete d-dimensional submanifold $B \subset \mathbb{R}^{d+k}$ with fibres diffeomorphic to $F \subset \mathbb{R}^k$, whose total space is embedded into an ε-neighbourhood of B. From this point of view, B takes the role of the curve and F that of the disc-shaped cross section of a conventional quantum waveguide. Our approach allows, among other things, for waveguides whose cross sections F are deformed along B and also the study of the Laplacian on the boundaries of such waveguides. By applying recent results on the adiabatic limit of Schrödinger operators on fibre bundles we show, in particular, that for small energies the dynamics and the spectrum of the Laplacian on M are reflected by the adiabatic approximation associated with the ground state band of the normal Laplacian. We give explicit formulas for the accordingly effective operator on $L^2(B)$ in various scenarios, thereby improving and extending many of the known results on quantum waveguides and quantum layers in $\mathbb{R}^3$.

1. Introduction

Quantum waveguides have been studied by physicists, chemists and mathematicians for many years now and the rate at which new contributions appear is still high (see e.g. [1,5,6,10,12,14,17,22,25] and references therein). Mathematically speaking, a conventional quantum waveguide corresponds to the study of the Dirichlet Laplacian on a thin tube around a smooth curve in $\mathbb{R}^3$. Of particular interest, are effects of the geometry of the tube on the spectrum of and the unitary group generated by the Laplacian. Similarly so-called quantum layers, i.e. the Laplacian on a thin layer around a smooth surface, have been studied [3,11,13]. The related problem of the constraining of a quantum particle to a neighbourhood of such a curve (or surface) by a steep potential

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rather than through the boundary condition was studied in [4,7,8,19–21,28]. Recently, progress has also been made on quantum waveguides and layers in magnetic fields [12,13,21].

There are obvious geometric generalisations of these concepts. One can consider the Dirichlet Laplacian on small neighbourhoods of d-dimensional submanifolds of $\mathbb{R}^{d+k}$ (see e.g. [18]), or of any $(d+k)$-dimensional Riemannian manifold. Another possibility is to look at the Laplacian on the boundary of such a submanifold, which, in the case of a conventional waveguide, is a cylindrical surface around a curve in $\mathbb{R}^3$. Beyond generalising to higher dimension and codimension, one could also ask for waveguides with cross sections that change their shape and size along the curve, or more generally along the submanifold around which the waveguide is modelled.

In the majority of mathematical works on quantum waveguides, with the exception of [22], such variations of the cross section along the curve must be excluded. The reason is that, physically speaking, localizing a quantum particle to a thin domain leads to large kinetic energies in the constrained directions, i.e. in the directions normal to the curve for a conventional waveguide, and that variations of the cross section lead to exchange of this kinetic energy between normal and tangent directions. However, the common approaches require that the Laplacian acts only on functions that have much smaller derivatives in the tangent directions than in the normal directions.

In this paper, we show how to cope with several of the possible generalisations mentioned above: (1) We consider general dimension and codimension of the submanifold along which the waveguide is modelled. (2) We allow for general variations of the cross sections along the submanifold and thus necessarily for kinetic energies of the same order in all directions, with possible exchange of energy between the tangent and normal directions. (3) We also include the case of "hollow" waveguides, i.e. the Laplacian on the boundary of a general "massive" quantum waveguide.

All of this is achieved by developing a suitable geometric framework for general quantum waveguides and by the subsequent application of recent results on the adiabatic limit of Schrödinger operators on fibre bundles [16]. As concrete applications, we will mostly emphasise geometric effects and explain, in particular, how the known effects of "bending" and "twisting" of waveguides in $\mathbb{R}^3$ (see [10] for a review) manifest themselves in higher dimensional generalised waveguides.

Before going into a more detailed discussion of our results and of the vast literature, let us review the main concepts in the context of conventional quantum waveguides in a geometric language that is already adapted to our subsequent generalisation. Moreover, it will allow us to explain the adiabatic structure of the problem within a simple example.

Consider a smooth curve $c : \mathbb{R} \to \mathbb{R}^3$ parametrised by arclength with bounded second derivative c''. For some $\varepsilon > 0$, we refer to the curve's ε-neighbourhood

$$\mathcal{T}^\varepsilon := \left\{ y \in \mathbb{R}^3 : \ \mathrm{dist}(y, B) \leq \varepsilon \right\} \subset \mathbb{R}^3$$

as the tube of a conventional waveguide. We assume, for ε small enough, that $\mathcal{T}^\varepsilon$ is non-self-intersecting, i.e. that one can map $\mathcal{T}^\varepsilon$ diffeomorphically onto the ε-tube in the normal bundle of B. The aim is to understand the Laplace operator Δ_{δ_3} on $L^2(\mathcal{T}^\varepsilon, \mathrm{d}\delta_3)$ with Dirichlet boundary conditions on $\mathcal{T}^\varepsilon$ in the asymptotic limit $\varepsilon \ll 1$. As different metrics will appear in the course of the discussion, we make the Euclidean metric δ_3 explicit in the Laplacian.

To make the following computations explicit, we pick an orthonormal frame along the curve. A natural choice is to start with an orthonormal basis (τ, e_1, e_2) at one point in B such that $\tau = c'$ is tangent and (e_1, e_2) are normal to the curve. Then, one obtains a (in this special case global) unique frame by parallel transport of (τ, e_1, e_2) along the curve B. This construction is sometimes called the relatively parallel-adapted frame [2]. The frame $(\tau(x), e_1(x), e_2(x))$ satisfies the differential equation

$$\begin{pmatrix} \tau' \\ e_1' \\ e_2' \end{pmatrix} = \begin{pmatrix} 0 & \kappa^1 & \kappa^2 \\ -\kappa^1 & 0 & 0 \\ -\kappa^2 & 0 & 0 \end{pmatrix} \begin{pmatrix} \tau \\ e_1 \\ e_2 \end{pmatrix} \tag{1.1}$$

with the components of the mean curvature vector $\kappa^\alpha : B \to \mathbb{R}$ $(\alpha = 1, 2)$ given by

$$\kappa^\alpha(x) := \langle \tau'(x), e_\alpha(x) \rangle_{\mathbb{R}^3} = \langle c''(x), e_\alpha(x) \rangle_{\mathbb{R}^3} .$$

The two normal vector fields $e_{1,2} : B \to \mathbb{R}^3$ form an orthonormal frame of B's normal bundle $\mathsf{N}B$. Hence, for $\varepsilon > 0$ small enough, there is a canonical identification of the ε-tube in the normal bundle denoted by

$$M^\varepsilon := \left\{ \left(x, n^1 e_1(x) + n^2 e_2(x)\right) \in \mathsf{N}B : \ (n^1)^2 + (n^2)^2 \le \varepsilon^2 \right\} \subset \mathsf{N}B$$

with the original ε-tube $\mathcal{T}^\varepsilon \subset \mathbb{R}^3$ via the map

$$\Phi : M^\varepsilon \to \mathcal{T}^\varepsilon, \quad \Phi : \left(x, n^1 e_1(x) + n^2 e_2(x)\right) \mapsto x + n^1 e_1(x) + n^2 e_2(x). \tag{1.2}$$

We will refer to $F_x^\varepsilon := M^\varepsilon \cap \mathsf{N}_x B$ as the cross section of M^ε and to $\Phi(F_x^\varepsilon)$ as the cross section of $\mathcal{T}^\varepsilon$ at $x \in B$.

To give somewhat more substance to the simple example, let us generalise the concept of a conventional waveguide already at this point. For a smooth function $f : B \to [f_-, f_+]$ with $0 < f_- < f_+ < \infty$ let

$$M_f^\varepsilon := \left\{ \left(x, n^1 e_1(x) + n^2 e_2(x)\right) \in \mathsf{N}B : \ (n^1)^2 + (n^2)^2 \le \varepsilon^2 f(x)^2 \right\}$$

be the tube with varying cross section F_x^ε, a disc of radius $\varepsilon f(x)$. This gives rise to a corresponding tube $\mathcal{T}_f^\varepsilon := \Phi(M_f^\varepsilon)$ in $\mathbb{R}^3$. To not overburden notation, we will drop the subscript f in the following, i.e. put $M^\varepsilon := M_f^\varepsilon$ and $\mathcal{T}^\varepsilon := \mathcal{T}_f^\varepsilon$.

By equipping M^ε with the pullback metric $g := \Phi^* \delta_3$, Φ becomes an isometry that can be lifted to a unitary operator $\widehat{\Phi} : L^2(\mathcal{T}^\varepsilon, \mathrm{d}\delta_3) \to L^2(M^\varepsilon, \mathrm{d}g)$ given by $\widehat{\Phi}\Psi = \Psi \circ \Phi$. Then, the Dirichlet Laplacian $-\Delta_{\delta_3}$ on (its dense domain in) $L^2(\mathcal{T}^\varepsilon, \mathrm{d}\delta_3)$ is unitarily equivalent to the Laplacian $\widehat{\Phi}(-\Delta_{\delta_3})\widehat{\Phi}^{-1}$ on $L^2(M^\varepsilon, \mathrm{d}g)$ with Dirichlet boundary conditions, which coincides with the Laplace–Beltrami operator $-\Delta_g$ associated with the pullback metric g. If (x, n^1, n^2) denote bundle coordinates associated with the orthonormal frame

$(e_1(x), e_2(x))$, the Laplacian Δ_g as differential operator on $C_0^\infty(M^\varepsilon)$ is given by

$$\Delta_g = \sum_{i,j=1}^{3} \frac{1}{\sqrt{|g|}} \partial_{q^i} \sqrt{|g|} g^{ij} \partial_{q^j}, \quad (q^1, q^2, q^3) = (x, n^1, n^2),$$

where $|g| := |\det(g)|$ and $g^{ij} := g(\mathrm{d}q^i, \mathrm{d}q^j)$ are the coefficients of the inverse metric tensor.

To obtain an explicit expression for Δ_g, we need to compute the pullback metric g on the tube M^ε. For the coordinate vector fields ∂_x and ∂_{n^α}, $\alpha \in \{1, 2\}$, one finds

$$\begin{aligned} \Phi_* \partial_x|_{(x,n)} &= \tfrac{\mathrm{d}}{\mathrm{d}x} \Phi\Big(\big(c(x), n^\alpha e_\alpha\big(c(x)\big)\big)\Big) = \tfrac{\mathrm{d}}{\mathrm{d}x}\Big(c(x) + n^\alpha e_\alpha\big(c(x)\big)\Big) \\ &= \tau(x) - n^\alpha \kappa^\alpha(x) \tau(x) = \big(1 - n \cdot \kappa(x)\big)\tau(x), \\ \Phi_* \partial_{n^\alpha}|_{(x,n)} &= \tfrac{\mathrm{d}}{\mathrm{d}n^\alpha} \Phi\Big(\big(c(x), n^\alpha e_\alpha\big(c(x)\big)\big)\Big) = \tfrac{\mathrm{d}}{\mathrm{d}n^\alpha}\Big(c(x) + n^\alpha e_\alpha\big(c(x)\big)\Big) \\ &= e_\alpha(x). \end{aligned}$$

Here, we used $c'(x) = \tau(x)$ and the differential equations (1.1). Knowing that (τ, e_1, e_2) is an orthonormal frame of $\mathsf{T}\mathbb{R}^3|_B$ with respect to δ_3, this yields

$$g(x, n) = \begin{pmatrix} (1 - n \cdot \kappa(x))^2 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

The Laplace–Beltrami operator on M^ε associated with g is thus

$$\Delta_g = \frac{1}{(1 - n \cdot \kappa)^2} \left(\partial_x^2 + \frac{n \cdot \kappa'}{1 - n \cdot \kappa}\, \partial_x \right) + \Delta_n - \frac{\kappa \cdot \nabla_n}{1 - n \cdot \kappa}$$

with the vertical Laplacian $\Delta_n = \nabla_n^2 = \partial_{n^1}^2 + \partial_{n^2}^2$.

As a next step we go over to a description where we blow up the tube in the normal directions and rescale the metric instead. More precisely, we dilate the fibres of $\mathsf{N}B$ using the diffeomorphism $\mathcal{D}_\varepsilon : M \to M^\varepsilon$, $(x, n) \mapsto (x, \varepsilon n)$, where $M := M^{\varepsilon=1}$. Equipping M with the pullback

$$\mathcal{D}_\varepsilon^* g(x, n) = \begin{pmatrix} (1 - \varepsilon n \cdot \kappa(x))^2 & 0 & 0 \\ 0 & \varepsilon^2 & 0 \\ 0 & 0 & \varepsilon^2 \end{pmatrix} \tag{1.3}$$

turns $\mathcal{D}_\varepsilon$ into an isometry with associated unitary lift

$$\widehat{\mathcal{D}}_\varepsilon : L^2(M, \mathrm{d}\mathcal{D}_\varepsilon^* g) \to L^2(M^\varepsilon, \mathrm{d}g), \quad \Psi \mapsto (\widehat{\mathcal{D}}_\varepsilon \Psi)(x, n) = \Psi\big(x, \tfrac{n}{\varepsilon}\big).$$

The unitarily equivalent Laplace–Beltrami operator on M associated with $\mathcal{D}_\varepsilon^* g$ is

$$\begin{aligned} \Delta_{\mathcal{D}_\varepsilon^* g} &= \widehat{\mathcal{D}}_\varepsilon^{-1} \Delta_g \widehat{\mathcal{D}}_\varepsilon \\ &= \frac{1}{(1 - \varepsilon n \cdot \kappa)^2} \left(\partial_x^2 + \frac{\varepsilon n \cdot \kappa'}{1 - \varepsilon n \cdot \kappa}\, \partial_x \right) + \varepsilon^{-2} \Delta_n - \frac{\kappa \cdot \varepsilon^{-1} \nabla_n}{1 - \varepsilon n \cdot \kappa}. \end{aligned}$$

In view of the factor ε^{-2} in front of the vertical Laplacian Δ_n, it is apparent that the limit $\varepsilon \ll 1$ leads to divergent kinetic energies in the transversal direction. For this reason, we rescale units of energy in such a way that the transverse energies are of order one by multiplying the full Laplacian with ε^2. On the geometric side, this corresponds to multiplying the metric with ε^{-2}, i.e. for $g^\varepsilon := \varepsilon^{-2}\mathcal{D}_\varepsilon^* g$ we have that

$$\Delta_{g^\varepsilon} = \varepsilon^2 \Delta_{\mathcal{D}_\varepsilon^* g} = \frac{\varepsilon^2}{(1-\varepsilon n\cdot\kappa)^2}\left(\partial_x^2 + \frac{\varepsilon n\cdot\kappa'}{1-\varepsilon n\cdot\kappa}\,\partial_x\right) + \Delta_n - \varepsilon\frac{\kappa\cdot\nabla_n}{1-\varepsilon n\cdot\kappa}.$$

Note that $-\Delta_{g^\varepsilon}$ on (its dense domain in) $L^2(M, \mathrm{d}\mathcal{D}_\varepsilon^* g)$ is unitarily equivalent to $-\Delta_{g^\varepsilon}$ on $L^2(M, \mathrm{d}g^\varepsilon)$, i.e. that changing the volume measure in the L^2-norm by a constant factor does not change the properties of the respective operators.

In a last step, we replace the volume measure $\mathrm{d}g^\varepsilon$ by the simpler density $\mathrm{d}\delta_3^\varepsilon$ of the appropriately scaled Euclidian metric $\delta_3^\varepsilon := \varepsilon^{-2}\mathcal{D}_\varepsilon^*\delta_3$. With

$$\mathrm{d}g^\varepsilon = \underbrace{(1-\varepsilon n\cdot\kappa(x))}_{=:\rho_\varepsilon(x,n)}\,\mathrm{d}\delta_3^\varepsilon,$$

the unitary map between the associated L^2-spaces is

$$\mathcal{M}_{\rho_\varepsilon} : L^2(M, \mathrm{d}g^\varepsilon) \to L^2(M, \mathrm{d}\delta_3^\varepsilon), \quad \Psi \mapsto \sqrt{\rho_\varepsilon}\Psi.$$

With this final unitary transformation, we arrive at the desired form of the Hamiltonian that serves as the starting point for the further analysis

$$H^\varepsilon := \mathcal{M}_{\rho_\varepsilon}\big(-\Delta_{g^\varepsilon}\big)\mathcal{M}_{\rho_\varepsilon}^{-1} = -\varepsilon^2\Delta_{\mathsf{H}} - \Delta_{\mathsf{V}} + \varepsilon^2 V_{\mathrm{bend}} - \varepsilon^3 S^\varepsilon.$$

Here, the leading order part is given by the sum of the horizontal Laplacian $\varepsilon^2\Delta_{\mathsf{H}} := \varepsilon^2\partial_x^2$ and the vertical Laplacian $\Delta_{\mathsf{V}} := \Delta_n$, which is just the Laplace–Beltrami operator associated with the metric δ_3^ε. The effects of the bending of the curve in the ambient space, i.e. its extrinsic geometry, are reflected in the so-called bending potential

$$V_{\mathrm{bend}} := -\frac{\kappa^2}{4\rho_\varepsilon^2} - \frac{\varepsilon n\cdot\kappa''}{2\rho_\varepsilon^3} - \frac{5(\varepsilon n\cdot\kappa')^2}{4\rho_\varepsilon^4} = -\frac{\kappa^2}{4} + \mathcal{O}(\varepsilon) \tag{1.4}$$

and the second-order differential operator

$$S^\varepsilon := \varepsilon^{-1}\partial_x \underbrace{(\rho_\varepsilon^{-2} - 1)}_{=2\varepsilon n\cdot\kappa + \mathcal{O}(\varepsilon^2)} \partial_x.$$

For sake of simplicity, we change our volume measure one last time from $\mathrm{d}\delta_3^\varepsilon$ to the Lebesgue measure $\mathrm{d}\delta_3 = \varepsilon\,\mathrm{d}\delta_3^\varepsilon$. Again, the change of the volume measure by a constant factor does not change the properties of the linear operators on the space.

In summary, the Hamiltonian H^ε is a self-adjoint operator with domain $D(H^\varepsilon) = W^2(M) \cap W_0^1(M) \subset L^2(M, \mathrm{d}\delta_3)$, that is unitarily equivalent to the initial Dirichlet Laplacian $-\varepsilon^2\Delta_{\delta^3}$ on the tube $\mathcal{T}^\varepsilon \subset \mathbb{R}^3$ (cf. Fig. 1). It splits into the horizontal Laplacian $\varepsilon^2\Delta_{\mathsf{H}} = \varepsilon^2\partial_x^2$, a symmetric operator on $D(H^\varepsilon)$, the vertical Laplacian $\Delta_{\mathsf{V}} = \Delta_n$, which is fibrewise the Dirichlet Laplacian on F_x, and an additional differential operator $\varepsilon H_1 := \varepsilon^2 V_{\mathrm{bend}} - \varepsilon^3 S^\varepsilon$, again a symmetric operator on $D(H^\varepsilon)$, that will be treated as a perturbation. This structure is reminiscent of the starting point for the Born–Oppenheimer approximation in molecular physics. There the x-coordinate(s) describe heavy

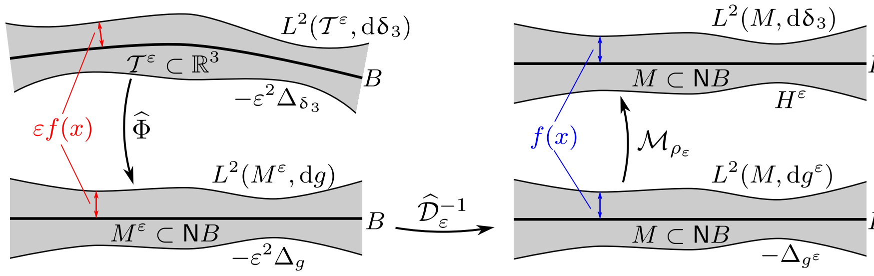

Figure 1. The successive unitary transformations that lead to the "adiabatic form" $H^\varepsilon = -\Delta_{\delta_3^\varepsilon} + \varepsilon H_1$ of the waveguide Hamiltonian: $\widehat{\Phi}$ implements the diffeomorphism into the normal bundle, $\widehat{\mathcal{D}}_\varepsilon^{-1}$ the blow up of the fibres, and $\mathcal{M}_{\rho_\varepsilon}$ a change of the volume measure

nuclei and ε^2 equals the inverse mass of the nuclei. The n-coordinates describe the electrons with mass of order one. In both cases, the vertical resp. electron operator depends on x: the vertical Laplacian Δ_{V} in the quantum waveguide Hamiltonian H^ε depends on $x \in B$ through the domain $F_x := F_x^{\varepsilon=1}$ and the electron operator in the molecular Hamiltonian depends on x through an interaction potential. This suggests to study the asymptotics $\varepsilon \ll 1$ for quantum waveguide Hamiltonians by the same methods that have been successfully developed for molecular Hamiltonians, namely by adiabatic perturbation theory (see e.g. [23,26]). The latter allows to separate slow and fast degrees of freedom in a systematic way. In the context of quantum waveguides, the tangent dynamics are slow compared to the frequencies of the normal modes.

To illustrate the adiabatic structure of the problem, let $\lambda_0(x) \sim f(x)^{-2}$ be the smallest eigenvalue of $-\Delta_{\mathsf{V}}$ on F_x and denote by $\phi_0(x) \in L^2(F_x)$ the corresponding normalised non-negative eigenfunction, the so-called ground state wave function. Let

$$P_0 L^2(M) := \left\{ \Psi(x,n) = \psi(x)\phi_0(x,n) : \ \psi \in L^2(B) \right\} \subset L^2(M)$$

be the subspace of local product states and P_0 the orthogonal projection onto this space. Now the restriction of H^ε to the subspace $P_0 L^2(M)$ is called the adiabatic approximation of H^ε on the ground state band and the associated adiabatic operator is defined by

$$H_{\mathrm{a}} := P_0 H^\varepsilon P_0. \tag{1.5}$$

A simple computation using

$$(P_0\Psi)(x,n) = \langle \phi_0(x,\cdot), \Psi(x,\cdot)\rangle_{L^2(F_x)} \phi_0(x,n)$$

and the unitary identification $W : P_0 L^2(M) \to L^2(B)$, $\psi(x)\phi_0(x,n^1,n^2) \mapsto \psi(x)$, shows that the adiabatic operator H_{a} can be seen as an operator acting only on functions on the curve B, given by

$$(WH_{\mathrm{a}}W^*\psi)(x) = \big(-\varepsilon^2\partial_x^2 + \lambda_0(x) + \varepsilon^2 V_{\mathrm{a}}(x) + \varepsilon^2 V^0_{\mathrm{bend}}(x)\big)\psi(x) \\ + \varepsilon^3 \int_{F_x} \phi_0(x,n)\big(S^\varepsilon(\phi_0\psi)\big)(x,n)\,\mathrm{d}n + \mathcal{O}(\varepsilon^3),$$

where $V_{\mathrm{a}}(x) := \|\partial_x\phi_0(x)\|^2_{L^2(F_x)}$ and $V^0_{\mathrm{bend}}(x) = -\frac{\kappa^2(x)}{4}$. As such it is a one-dimensional Schrödinger-type operator with potential function $\lambda_0(x) + \mathcal{O}(\varepsilon^2)$ and the asymptotic limit $\varepsilon \ll 1$ corresponds to the semi-classical limit. This analogy shows that, in general, $-\varepsilon^2\partial_x^2$ cannot be considered small compared to $\lambda_0(x)$, despite the factor of ε^2. To see this, observe that all eigenfunctions ψ^ε (and also all solutions of the corresponding time-dependent Schrödinger equation) are necessarily ε-dependent with $\|\varepsilon\partial_x\psi^\varepsilon\|^2 \gg \varepsilon^2$, unless $\lambda_0(x) \equiv C$ for some constant $C \geq 0$. To be more explicit, assume that $\lambda_0(x) \approx \omega^2(x-x_0)^2$ near a global minimum at x_0. Then, the lowest eigenvalues of H_{a} are $e_\ell = \lambda_0(x_0) + \varepsilon\omega(1+2\ell) + \mathcal{O}(\varepsilon^2)$ for $\ell = 0, 1, 2, \ldots$. While the level spacing of order ε is small compared to λ_0, it is large compared to the energy scale of order ε^2 of the geometric potentials. And for states ψ^ε with $\ell \sim \varepsilon^{-1}$, the kinetic energy $\|\varepsilon\partial_x\psi^\varepsilon\|^2$ in the tangential direction is of order one.

However, the majority of mathematical works on the subject considers the situation where $\|\varepsilon\partial_x\psi^\varepsilon\|^2$ is of order ε^2. Clearly this only yields meaningful results if one assumes λ_0 to be constant. But this, in turn, puts strong constraints on the possible geometries of the waveguide, which we avoid in the present paper.

Now the obvious mathematical question is: *To what extent and in which sense do the properties of the adiabatic operator H_{a} reflect the corresponding properties of H^ε?* This question was answered in great generality in [15,16] and we will translate these results to our setting of generalised quantum waveguides in Sect. 3. Roughly speaking, Theorem 3.3 states that the low-lying eigenvalues of H_{a} approximate those of H^ε up to errors of order ε^3 in general, and up to order ε^4 in the special case where λ_0 is a non-negative constant. In the latter case, the order ε^3 terms in H_{a} turn out to be significant as well.

Our main new contribution in this work is to introduce the concept of generalised quantum waveguides in Sect. 2 and to compute explicitly the adiabatic operator for such generalised waveguides to all significant orders. For massive quantum waveguides, which are basically "tubes" with varying cross sections modelled over submanifolds of arbitrary dimension and codimension, this is done in Sect. 4. There we follow basically the same strategy as in the simple example given in the present section. We obtain general expressions for the adiabatic operator, from which we determine the relevant terms for different energy scales. Though the underlying calculations of geometric quantities have been long known [27], the contribution of S^ε has usually been neglected, because at the energy scale of ε^2 it is of lower order than V_{bend}. This changes, however, on the natural energy scale of the example M_f with non-constant f, where they may be of the same order, as we see in Sect. 4.4.3. The contribution of the bending potential is known to be non-positive in dimensions $d = 1$ or $d = 2$ [3,6], while it has no definite sign in higher dimensions [27].

It was stressed in [6] that this leads to competing effects of bending and the non-negative "twisting potential" in quantum waveguides whose cross sections F_x are all isometric but not rotationally invariant and twist along the curve relative to the parallel frame. The generalisation of this twisting potential is the adiabatic potential V_{a}, which is always non-negative and of the same order as V_{bend}. Using this general framework we generalise the concept of "twisted" waveguides to arbitrary dimension and codimension in Sect. 4.4.2.

In Sect. 5, we finally consider hollow waveguides, which are the boundaries of massive waveguides. So far there seems to be no results on these waveguides in the literature and the adiabatic operator derived in Sect. 5.2 is completely new. For hollow waveguides, the vertical operator is essentially the Laplacian on a compact manifold without boundary and thus its lowest eigenvalue vanishes identically, $\lambda_0(x) \equiv 0$. The adiabatic operator on $L^2(B)$ is quite different from the massive case. Up to errors of order ε^3, it is the sum of the Laplacian on B and an effective potential given in (5.10). For the special case of the boundary of M_f^ε discussed above, this potential is given by

$$\varepsilon^2 \left[\tfrac{1}{2}\partial_x^2 \log\bigl(2\pi f(x)\bigr) + \tfrac{1}{4}\bigl|\partial_x \log\bigl(2\pi f(x)\bigr)\bigr|^2\right] = \varepsilon^2 \left[\tfrac{1}{2}\tfrac{f''}{f} - \tfrac{1}{4}\bigl(\tfrac{f'}{f}\bigr)^2\right],$$

which, in contrast to massive waveguides, is independent of the curvature κ and depends only on the rate of change of $\mathrm{Vol}(\partial F_x) = 2\pi f(x)$. One can check for explicit examples that a local constriction in the tube, e.g. for $f(x) = 2 - \frac{1}{1+x^2}$, leads to an effective potential with wells. Thus, constrictions can support bound states on the surface of a tube.

2. Generalised Quantum Waveguides

In this part, we give a precise definition of what we call generalised quantum waveguides. In view of the example discussed in Sect. 1, the ambient space $\mathbb{R}^3$ is replaced by the $(d+k)$-dimensional Euclidean space and the role of the curve is played by a smooth, complete, embedded d-dimensional submanifold $B \subset \mathbb{R}^{d+k}$. There will be a slight change of perspective, as a generalised waveguide is not initially defined as a subset of $\mathbb{R}^{d+k}$ but constructed from a set M contained in a neighbourhood of the zero section in the normal bundle $\mathsf{N}B$, which then can be diffeomorphically mapped to a tubular neighbourhood of $B \subset \mathbb{R}^{d+k}$. We will again call $F_x = M \cap \mathsf{N}_x B$ the cross section of the quantum waveguide at the point $x \in B$ and essentially assume that F_x and F_y are diffeomorphic for $x, y \in B$. This allows for more general deformations of the cross sections as one moves along the base, where in Sect. 1 we only considered scaling by the function f.

For the following considerations, we assume that there exists a tubular neighbourhood $B \subset \mathcal{T}^r \subset \mathbb{R}^{d+k}$ with globally fixed radius, i.e. there is $r > 0$ such that normals to B of length less than r do not intersect. More precisely, we assume that the map

$$\Phi : \mathsf{N}B \to \mathbb{R}^{d+k}, \quad (x, \nu) \mapsto x + \nu,$$

restricted to

$$\mathsf{N}B^r := \big\{(x,\nu) \in \mathsf{N}B : \ \|\nu\|_{\mathbb{R}^{d+k}} < r\big\} \subset \mathsf{N}B$$

is a diffeomorphism to its image $\mathcal{T}^r$. By equipping $\mathsf{N}B^r$ with the pullback metric $G := \Phi^*\delta_{d+k}$, the tubular neighbourhood $\mathcal{T}^r$ of $B \subset \mathbb{R}^{d+k}$ is isometric to $\mathsf{N}B^r$ and all the analysis can be done in the normal bundle. In particular, the scaled waveguide is defined in a straightforward way by $M^\varepsilon := \{(x,\nu) \in \mathsf{N}B : \ (x, \frac{\nu}{\varepsilon}) \in M\}$ for $0 < \varepsilon \leq 1$ starting from the unscaled waveguide $M = M^{\varepsilon=1} \subset \mathsf{N}B^r$. As we saw in Sect. 1, it is more convenient to stay on the unscaled waveguide M and to scale the metric as $G^\varepsilon := \varepsilon^{-2}\mathcal{D}_\varepsilon^* G$ instead, where $\mathcal{D}_\varepsilon : (x,\nu) \mapsto (x, \varepsilon\nu)$ is the dilatation of the fibres in $\mathsf{N}B$. Note that G^ε coincides with g^ε for "massive" waveguides (cf. Definition 2.2) as considered in Sect. 1. By construction, the Laplace–Beltrami operator $-\Delta_{G^\varepsilon}$ on the tubular neighbourhood $\mathsf{N}B^r$ in the normal bundle is again equivalent to the Euclidian Laplacian $-\varepsilon^2\Delta_{\delta_{d+k}}$ on the scaled tubular neighbourhood $\mathcal{T}^{\varepsilon r} \subset \mathbb{R}^{d+k}$, in the sense that for functions $\Psi \in C_0^\infty(\mathsf{N}B^r)$ it holds that

$$-\Delta_{G^\varepsilon}\Psi = \widehat{\mathcal{D}}_\varepsilon^{-1}\widehat{\Phi}\big(\varepsilon^2\Delta_{\delta_{d+k}}\big)\widehat{\Phi}^{-1}\widehat{\mathcal{D}}_\varepsilon\Psi.$$

The same holds for the restrictions of the operators to $M \subset \mathsf{N}B^r$ and to $\Phi(M^\varepsilon) \subset \mathbb{R}^{d+k}$, respectively.

Definition 2.1. Let $B \subset \mathbb{R}^{d+k}$ be a smooth, complete, embedded d-dimensional submanifold with tubular neighbourhood $\mathcal{T}^r \subset \mathbb{R}^{d+k}$ possessing a globally fixed radius $r > 0$, and F be a compact manifold of dimension $\dim(F) \leq k$ with smooth boundary.

Let $M \subset \mathsf{N}B^r$ be a connected subset that is a fibre bundle with projection $\pi_M : M \to B$ and typical fibre F such that the diagram

$$\begin{array}{ccc} M & \hookrightarrow & \mathsf{N}B^r \\ \downarrow{\scriptstyle \pi_M} & & \downarrow{\scriptstyle \pi_{\mathsf{N}B}} \\ B & \xrightarrow[\mathrm{id}_B]{} & B \end{array}$$

commutes. We then call the pair (M, g^ε), with the scaled pullback metric

$$g^\varepsilon := G^\varepsilon|_{\mathsf{T}M} \in \mathcal{T}_2^0(M),$$

a *generalised quantum waveguide.*

It immediately follows from the commutative diagram that the cross sections F_x coincide with the fibres $\pi_M^{-1}(x)$ given by the fibre bundle structure. From now on, we will usually refer to this object simply as the fibre of M over x. Although other geometries are conceivable, the most interesting examples of generalised waveguides are given by subsets $M \subset \mathsf{N}B^r$ of codimension zero and their boundaries. In the following, we will only treat these two cases and distinguish them by the following terminology:

Definition 2.2. Let $F \to M \xrightarrow{\pi_M} B$ be a generalised quantum waveguide as in Definition 2.1.

1. We call M *massive* if F is the closure of an open, bounded and connected subset of $\mathbb{R}^k$ with smooth boundary.
2. We call M *hollow* if $\dim(F) > 0$ and there exists a massive quantum waveguide $\mathring{F} \to \mathring{M} \xrightarrow{\pi_{\mathring{M}}} B$ such that $M = \partial\mathring{M}$.

This definition implies $\pi_M = \pi_{\mathring{M}}|_M$, i.e. each fibre $F_x = \pi_M^{-1}(x)$ of a hollow quantum waveguide is the boundary of $\mathring{F}_x$, the fibre of the related massive waveguide $\mathring{M}$.

We denote by $\mathsf{V}M := \ker(\pi_{M*}) \subset \mathsf{T}M$ the vertical subbundle of $\mathsf{T}M$. Its elements are vectors that are tangent to the fibres of M. We refer to the orthogonal complement of $\mathsf{V}M$ (with respect to $g := g^{\varepsilon=1}$) as the horizontal subbundle $\mathsf{H}M \cong \pi_M^*(\mathsf{T}B)$. Clearly

$$\mathsf{T}M = \mathsf{H}M \oplus \mathsf{V}M, \tag{2.1}$$

and this decomposition will turn out to be independent of ε. That is, the decomposition $\mathsf{T}M = \mathsf{H}M \oplus \mathsf{V}M$ is orthogonal for every $\varepsilon > 0$. Furthermore, we will see [Lemma 4.1 and Eq. (4.6) for the massive case, Eq. (5.5) for hollow waveguides] that the scaled pullback metric is always of the form

$$g^\varepsilon = \varepsilon^{-2}(\pi_M^* g_B + \varepsilon h^\varepsilon) + g_F, \tag{2.2}$$

where

- $g_B := \delta_{d+k}|_{\mathsf{T}B} \in \mathcal{T}_2^0(B)$ is the induced Riemannian metric on the submanifold B,
- $h^\varepsilon \in \mathcal{T}_2^0(M)$ is a symmetric (but not non-degenerate) tensor with $h^\varepsilon(V, \cdot) = 0$ for any vertical vector field V,
- $g_F := g^\varepsilon|_{\mathsf{V}M}$ is the ε-independent restriction of the scaled pullback metric to the vertical subbundle.

Thus, if we define for any vector field $X \in \Gamma(\mathsf{T}B)$ its unique horizontal lift $X^{\mathsf{H}M} \in \Gamma(\mathsf{H}M)$ by the relation $\pi_{M*}X^{\mathsf{H}M} = X$, we have

$$\begin{aligned} g^\varepsilon(X^{\mathsf{H}M}, Y^{\mathsf{H}M}) &= \varepsilon^{-2}\big(g_B(X,Y) + \varepsilon h^\varepsilon(X^{\mathsf{H}M}, X^{\mathsf{H}M})\big), \\ g^\varepsilon(X^{\mathsf{H}M}, V) &= 0, \\ g^\varepsilon(V, W) &= g_F(V, W) \end{aligned}$$

for all $X, Y \in \Gamma(\mathsf{T}B)$ and $V, W \in \Gamma(\mathsf{V}M)$.

By dropping the term h^ε, we arrive at the metric

$$g_{\mathrm{s}}^\varepsilon := \varepsilon^{-2}\pi_M^* g_B + g_F$$

that turns π_M into a Riemannian submersion, i.e. π_{M*} into an isometry from $\mathsf{H}M$ to $\mathsf{T}B$ (up to a factor ε^{-1}). For this reason, we call $g_{\mathrm{s}}^\varepsilon$ the scaled submersion metric.

Example. (a) In Sect. 1, we considered a massive waveguide $M = M_f$ with $d = 1$ and $k = 2$. The typical fibre was given by $F = \mathbb{D}^2 \subset \mathbb{R}^2$. Using the bundle coordinates (x, n^1, n^2) induced by (1.2), the scaled pullback metric was [cf. (1.3)]

$$g^\varepsilon := \begin{pmatrix} \varepsilon^{-2}(1-\varepsilon n\cdot\kappa)^2 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 1\end{pmatrix}$$
$$= \varepsilon^{-2}\Big[\underbrace{\mathrm{d}x^2}_{=g_B} + \varepsilon\underbrace{\left(-2(n\cdot\kappa)+\varepsilon(n\cdot\kappa)^2\right)\mathrm{d}x^2}_{=h^\varepsilon}\Big] + \underbrace{\mathrm{d}(n^1)^2+\mathrm{d}(n^2)^2}_{=:\mathrm{d}n^2=g_F}$$

Moreover, the scaled submersion metric g_s^ε is just the scaled Euclidian metric $\delta_3^\varepsilon = \varepsilon^{-2}\,\mathrm{d}x^2 + \mathrm{d}n^2$.

(b) The typical fibre of the associated hollow waveguide is $\mathbb{S}^1 = \partial\mathbb{D}^2 \subset \mathbb{R}^2$ and we compute the form of the restricted metric g^ε in Sect. 5 (cf. Example 5.1).

After having introduced the geometry of a generalised quantum waveguide (M, g^ε), we now analyse the Laplace–Beltrami operator $-\Delta_{g^\varepsilon}$ with Dirichlet boundary conditions. The boundary condition is of course vacuous if M is hollow since $\partial M = \emptyset$ in that case. As in Sect. 1, the key step for splitting the operator $-\Delta_{g^\varepsilon}$ into a horizontal and a vertical part at leading order is an appropriate change of the volume measure. Therefore, let

$$\rho_\varepsilon := \frac{\mathrm{d}g^\varepsilon}{\mathrm{d}g_\mathrm{s}^\varepsilon} \tag{2.3}$$

be the relative volume density of g^ε and g_s^ε, respectively, and

$$\mathcal{M}_{\rho_\varepsilon} : L^2(M, \mathrm{d}g^\varepsilon) \to L^2(M, \mathrm{d}g_\mathrm{s}^\varepsilon), \quad \Psi \mapsto \mathcal{M}_{\rho_\varepsilon}\Psi = \sqrt{\rho_\varepsilon}\Psi,$$

the according unitary multiplication operator. The transformed Laplacian then reads

$$H^\varepsilon = \mathcal{M}_{\rho_\varepsilon}\big(-\Delta_{g^\varepsilon}\big)\mathcal{M}_{\rho_\varepsilon}^{-1} = -\varepsilon^2\Delta_\mathsf{H} - \Delta_\mathsf{V} + \varepsilon^2 V_\mathrm{bend} - \varepsilon^3 S^\varepsilon.$$

Again we consider H^ε as a self-adjoint operator on the ε-independent space $L^2(M, \mathrm{d}g_\mathrm{s})$ with domain $D(H^\varepsilon) = W^2(M, g_\mathrm{s}) \cap W_0^1(M, g_\mathrm{s})$, where $g_\mathrm{s} := g_\mathrm{s}^{\varepsilon=1} = \pi_M^* g_B + g_F$ is the unscaled version of the submersion metric.

Remark 2.3. (a) The Sobolev space $W^k(M, g_\mathrm{s})$, $k \in \mathbb{N}$, may be defined globally as those $\Psi \in L^2(M, \mathrm{d}g_\mathrm{s})$ such that for $1 \le l \le k$ the covariant derivatives $\nabla^l\Psi$ with respect to g_s are L^2-sections of $(\mathsf{T}^*M)^{\otimes l}$. $W_0^k(M, g_\mathrm{s})$ is the closure of $C_0^\infty(M \setminus \partial M)$ in $W^k(M, g_\mathrm{s})$. In the following we will use Sobolev spaces associated with the Riemannian manifolds (M, g_s), (B, g_B), and (F_x, g_{F_x}) without making the dependence on the metric explicit in the notation.

(b) Since we will consider waveguides of bounded geometry (see Definition 3.1), the total space M, the base B, and the fibres F_x are manifolds of bounded geometry in the sense of Schick [24] (see [15, Proposition A.4]). For manifolds of bounded geometry, the previous definition of Sobolev spaces is equivalent to using the sum of locally defined norms obtained from an atlas $\{(U_\nu, \theta_\nu, \chi_\nu)\}_{\nu\in\mathbb{Z}}$ of "normal" coordinate charts $\theta_\nu : U_\nu \to \mathbb{R}^n$ with subordinate partition of unity χ_ν (see [24, Chapter 3]):

$$\|\Psi\|_{W^k}^2 := \sum_{\nu\in\mathbb{Z}} \|\theta_{\nu *}(\chi_\nu\Psi)\|_{W^k(\theta_\nu(U_\nu))}^2 .$$

Different choices of normal coordinates yield equivalent norms.

The horizontal Laplacian is defined by its quadratic form

$$\begin{aligned}\langle \Psi, -\Delta_{\mathsf{H}}\Psi\rangle &= \int_M \pi_M^* g_B\big(\operatorname{grad}_{g_s}\overline{\Psi}, \operatorname{grad}_{g_s}\Psi\big)\, \mathrm{d}g_s\\ &= \int_M g_s\big(\operatorname{grad}_{g_s}\overline{\Psi}, \mathrm{P}^{\mathsf{H}M}\operatorname{grad}_{g_s}\Psi\big)\, \mathrm{d}g_s,\end{aligned}$$

where $\mathrm{P}^{\mathsf{H}M}$ denotes the orthogonal projection to $\mathsf{H}M$, so integration by parts yields (see also Sect. 4.2)

$$\Delta_{\mathsf{H}} = \operatorname{div}_{g_s}\mathrm{P}^{\mathsf{H}M}\operatorname{grad}_{g_s}. \tag{2.4}$$

It is a symmetric operator on $D(H^\varepsilon)$. The vertical operator is given on each fibre F_x by the Laplace–Beltrami operator

$$\Delta_{\mathsf{V}}|_{F_x} := \Delta_{g_{F_x}}$$

with Dirichlet boundary conditions. It is self-adjoint on the domain $W^2(F_x)\cap W_0^1(F_x)$. The bending potential

$$\begin{aligned}\varepsilon^2 V_{\text{bend}} &= \tfrac{1}{2}\operatorname{div}_{g_s}\operatorname{grad}_{g^\varepsilon}(\log\rho_\varepsilon) + \tfrac{1}{4}g^\varepsilon(\mathrm{d}\log\rho_\varepsilon, \mathrm{d}\log\rho_\varepsilon)\\ &= \tfrac{1}{2}(\varepsilon^2\Delta_{\mathsf{H}} + \Delta_{\mathsf{V}})(\log\rho_\varepsilon) + \tfrac{1}{4}g_F(\mathrm{d}\log\rho_\varepsilon, \mathrm{d}\log\rho_\varepsilon) + \mathcal{O}(\varepsilon^4)\end{aligned} \tag{2.5}$$

is a by-product of the unitary transformation M_{ρ_ε} and the second-order differential operator

$$S^\varepsilon : \Psi \mapsto S^\varepsilon\Psi := \varepsilon^{-3}\operatorname{div}_{g_s}(g^\varepsilon - g_s^\varepsilon)(\mathrm{d}\Psi, \cdot)$$

accounts for the corrections to g_s^ε.

3. Adiabatic Perturbation Theory

In this section, we show that the adiabatic operator H_a approximates essential features of generalised quantum waveguide Hamiltonians H^ε, such as its unitary group and its spectrum. This motivates the derivation of explicit expansions of H_a in the subsequent sections. In this work, we will only consider the ground state band $\lambda_0(x)$ and pay special attention to the behaviour of H^ε for small energies. This, as we will show, allows to view H_a as an operator on $L^2(B)$. The results of this section were derived in [15,16] in more generality.

For a massive quantum waveguide set

$$H_F := -\Delta_{\mathsf{V}} \tag{massive}$$

and for a hollow waveguide

$$\begin{aligned}H_F &:= \mathcal{M}_{\rho_\varepsilon}(-\Delta_{\mathsf{V}})\mathcal{M}_{\rho_\varepsilon}^{-1}\\ &= -\Delta_{\mathsf{V}} + \tfrac{1}{2}\Delta_{\mathsf{V}}(\log\rho_\varepsilon) + \tfrac{1}{4}g_F(\mathrm{d}\log\rho_\varepsilon, \mathrm{d}\log\rho_\varepsilon).\end{aligned} \tag{hollow}$$

Let $\lambda_0(x) := \min\sigma(H_{F_x})$ be the smallest eigenvalue of the fibre operator H_F acting on the fibre over x. For hollow waveguides, we have no boundary and $\lambda_0 \equiv 0$ with the eigenfunction

$$\begin{aligned}\phi_0 &= \frac{\mathcal{M}_{\rho_\varepsilon}\pi_M^* \operatorname{Vol}(F_x)^{-1/2}}{\left\|\mathcal{M}_{\rho_\varepsilon}\pi_M^* \operatorname{Vol}(F_x)^{-1/2}\right\|_{L^2(F_x,\mathrm{d}g_F)}}\\ &= \sqrt{\rho_\varepsilon}\left(\int_{F_x}\rho_\varepsilon \,\mathrm{d}g_F\right)^{-1/2} = \pi_M^* \operatorname{Vol}(F_x)^{-1/2} + \mathcal{O}(\varepsilon).\end{aligned}$$

In the massive case, we have $\lambda_0 > 0$ and denote by $\phi_0(x,\cdot)$ the uniquely determined positive normalised eigenfunction of H_{F_x} with eigenvalue $\lambda_0(x)$. Let P_0 be the orthogonal projection in $L^2(M)$ defined by

$$(P_0\Psi)(x,\nu) = \phi_0\big(x,\nu\big)\int_{F_x}\phi_0\big(x,\cdot\big)\Psi(x,\cdot)\,\mathrm{d}g_F.$$

The image of this projection is the subspace $L^2(B)\otimes \operatorname{span}(\phi_0)\cong L^2(B)$ of $L^2(M)$. The function ϕ_0 and its derivatives, both horizontal and vertical, are uniformly bounded in ε. Thus, the action of the horizontal Laplacian $-\varepsilon^2\Delta_{\mathsf{H}}$ on ϕ_0 gives a term of order ε and

$$[H^\varepsilon, P_0]P_0 = [H^\varepsilon - H_F, P_0]P_0 = \mathcal{O}(\varepsilon) \tag{3.1}$$

as an operator from $D(H^\varepsilon)$ to $L^2(M)$. Since this expression equals $(H^\varepsilon - H_{\mathrm{a}})P_0$, this justifies the adiabatic approximation (1.5) for states in the image of P_0. However, the error is of order ε, while interesting effects of the geometry, such as the potentials V_{a} and V_{bend} discussed in Sect. 1, are of order ε^2. Because of this, it is desirable to construct also a super-adiabatic approximation, consisting of a modified projection $P_\varepsilon = P_0 + \mathcal{O}(\varepsilon)\in\mathcal{L}(L^2(M))\cap\mathcal{L}(D(H^\varepsilon))$ and an intertwining unitary U_ε with $P_\varepsilon U_\varepsilon = U_\varepsilon P_0$, such that the effective operator

$$H_{\mathrm{eff}} := P_0 U_\varepsilon^{-1} H^\varepsilon U_\varepsilon P_0$$

provides a better approximation of H^ε than H_{a} does. It then turns out that the approximation provided by H_{a} can be shown to be more accurate than expected from (3.1) using the unitary U_ε.

Such approximations can be constructed and justified if the geometry of (M, g^ε) satisfies some uniformity conditions. Here, we only spell out the conditions relevant to our case, for a comprehensive discussion see [15].

Definition 3.1. The generalised quantum waveguide (M, g^ε) is a *waveguide of bounded geometry* if the following conditions are satisfied:

1. The manifold (B, g_B) is of bounded geometry. This means it has positive injectivity radius and for every $k\in\mathbb{N}$ there exists a constant $C_k > 0$ such that

$$g_B(\nabla^k R, \nabla^k R)\le C_k,$$

where R denotes the curvature tensor of B and ∇, g_B are the connections and metrics induced on the tensor bundles over B.

2. The fibre bundle $(M, g)\xrightarrow{\pi_M}(B, g_B)$ is uniformly locally trivial. That is, there exists a Riemannian metric g_0 on F such that for every $x\in B$ and metric ball $B(r,x)$ of radius $r < r_{\mathrm{inj}}(B)$ there is a trivialisation $\Omega_{x,r}$: $(\pi_M^{-1}(B(x,r)), g)\to (B(x,r)\times F, g_B\times g_0)$, and the tensors $\Omega_{x,r}^*$ and $\Omega_{x,r*}$ and all their covariant derivatives are bounded uniformly in x.

3. The embeddings $(M,g) \hookrightarrow (\mathsf{N}B, G)$ and $(B, g_B) \hookrightarrow \mathbb{R}^{d+k}$ are bounded with all their derivatives.

These conditions are trivially satisfied for compact manifolds M and many examples, such as "asymptotically straight" or periodic waveguides. The existence result for the super-adiabatic approximation can be formulated as follows.

Theorem 3.2 [16]. *Let M be a waveguide of bounded geometry and set $\Lambda := \inf_{x\in B} \min(\sigma(H_{F_x}) \setminus \lambda_0)$. For every $N \in \mathbb{N}$, there exist a projection P_ε and a unitary U_ε in $\mathcal{L}(L^2(M)) \cap \mathcal{L}(D(H^\varepsilon))$, intertwining P_0 and P_ε, such that for every $\chi \in C_0^\infty\big((-\infty,\Lambda),[0,1]\big)$, satisfying $\chi^p \in C_0^\infty\big((-\infty,\Lambda),[0,1]\big)$ for every $p \in (0,\infty)$, we have*

$$\big\|H^\varepsilon \chi(H^\varepsilon) - U_\varepsilon H_{\mathrm{eff}} \chi(H_{\mathrm{eff}}) U_\varepsilon^{-1}\big\| = \mathcal{O}(\varepsilon^N).$$

In particular, the Hausdorff distance between the spectra of H^ε and H_{eff} is small, i.e. for every $\delta > 0$:

$$\operatorname{dist}\big(\sigma(H^\varepsilon) \cap (-\infty, \Lambda-\delta], \sigma(H_{\mathrm{eff}}) \cap (-\infty, \Lambda-\delta]\big) = \mathcal{O}(\varepsilon^N).$$

For $N = 1$, we can choose $P_\varepsilon = P_0$, so at first sight the approximation of H^ε by H_{a} yields errors of order ε. More careful inspection shows that for $N > 1$ we have $H_{\mathrm{a}} - H_{\mathrm{eff}} = \mathcal{O}(\varepsilon^2)$ as an operator from $W^2(B)$ to $L^2(M)$, so the statement on the spectrum holds for H_{a} with an error of order ε^2. This improvement over (3.1) relies on the existence of U_ε for a better choice of trial states. Close to the ground state, the approximation is even more accurate.

Theorem 3.3 [16]. *Let M be a waveguide of bounded geometry, $\Lambda_0 := \inf_{x\in B} \lambda_0(x)$ and $0 < \alpha \le 2$. Then for every $C > 0$*

$$\operatorname{dist}\big(\sigma(H^\varepsilon) \cap (-\infty, \Lambda_0 + C\varepsilon^\alpha], \sigma(H_{\mathrm{a}}) \cap (-\infty, \Lambda_0 + C\varepsilon^\alpha]\big) = \mathcal{O}(\varepsilon^{2+\alpha/2}).$$

Assume, in addition, that $\Lambda_0 + C\varepsilon^\alpha$ is strictly below the essential spectrum of H_{a} in the sense that for some $\delta > 0$ and ε small enough the spectral projection $\mathbf{1}_{(-\infty,\Lambda_0+(C+\delta)\varepsilon^\alpha]}(H_{\mathrm{a}})$ has finite rank. Then, if $\mu_0 < \mu_1 \le \cdots \le \mu_K$ are all the eigenvalues of H_{a} below $\Lambda_0 + C\varepsilon^\alpha$, H^ε has at least $K+1$ eigenvalues $\nu_0 < \nu_1 \le \cdots \le \nu_K$ below its essential spectrum and

$$|\mu_j - \nu_j| = \mathcal{O}(\varepsilon^{2+\alpha})$$

for $j \in \{0,\ldots,K\}$.

The natural energy scale α to consider this theorem would be the spacing of eigenvalues of H_{a}. This of course depends on the specific situation. If λ_0 is constant, we will see that $\alpha = 2$ is a natural choice. In the somewhat more generic case in which the eigenband $\lambda_0(x)$ has a global and non-degenerate minimum, as in the example of the waveguide M_f in Sect. 1, the lowest eigenvalues of H_{a} will behave like those of an harmonic oscillator and $\alpha = 1$ is the correct choice of scale. In this case, the set $(-\infty, \Lambda_0 + C\varepsilon^2] \cap \sigma(H_{\mathrm{a}})$ will just be empty for ε small enough and thus by the theorem there is no spectrum of H^ε in this interval.

We remark that results can be obtained also for energies higher than Λ and projections to other eigenbands than λ_0. The relevant condition is that they are separated from the rest of the spectrum of H_F by a local gap. For λ_0, this is a consequence of the bounded geometry of M (see [16, Proposition 4.1]). The approximation of spectra is not mutual as for low energies, but there is always spectrum of H^ε near that of H_{eff} (see [16, Corollary 2.4]).

From now on, we will focus on analysing the adiabatic operator. In particular, we will see how the geometry of the waveguide enters into this operator and its expansion up to order ε^4, which is relevant for small energies irrespective of the super-adiabatic corrections by Theorem 3.3. We now give a general expression for H_{a} from which we will derive the explicit form for various specific situations. First group the terms of H^ε in such a way that

$$H^\varepsilon = -\varepsilon^2 \Delta_{\mathsf{H}} + H_F + \varepsilon H_1,$$

by taking

$$\begin{aligned} H_1 &= -\varepsilon^2 S^\varepsilon + \varepsilon V_{\text{bend}}, && \text{(massive)} \\ H_1 &= -\varepsilon^2 S^\varepsilon + \varepsilon V_{\text{bend}} - \varepsilon^{-1}\big(\tfrac{1}{2}\Delta_{\mathsf{V}}(\log\rho_\varepsilon) + \tfrac{1}{4} g_F\big(\mathrm{d}\log\rho_\varepsilon, \mathrm{d}\log\rho_\varepsilon\big)\big) && \\ &= -\varepsilon^2 S^\varepsilon + \underbrace{\tfrac{\varepsilon}{2}\Delta_{\mathsf{H}}(\log\rho_\varepsilon) + \mathcal{O}(\varepsilon^3)}_{=:\varepsilon\tilde V_{\text{bend}}}. && \text{(hollow)} \end{aligned}$$

Projecting this expression with P_0 as in Eq. (1.5) gives $H_F P_0 = \lambda_0 P_0$ and

$$P_0 \Delta_{\mathsf{H}} P_0 = \Delta_{g_B} + \underbrace{\tfrac{1}{2}\mathrm{tr}_{g_B}(\nabla^B \bar\eta) - \int_{F_x} \pi_M^* g_B(\mathrm{grad}_{g_{\mathrm{s}}}\phi_0, \mathrm{grad}_{g_{\mathrm{s}}}\phi_0)\, \mathrm{d}g_F}_{=:-V_{\mathrm{a}}}, \quad (3.2)$$

where ∇^B is the Levi-Cività connection of g_B, $\bar\eta$ is the one-form

$$\bar\eta(X) := \int_{F_x} |\phi_0|^2 g_B(\pi_{M*}\eta_F, X)\mathrm{d}g_F$$

and η_F is the mean curvature vector of the fibres [see Eq. (4.8)]. The derivation for the projection of Δ_{H} can be found in [15, Chapter 3].

Altogether we have the expression

$$H_{\mathrm{a}} = -\varepsilon^2 \Delta_{g_B} + \lambda_0 + \varepsilon^2 V_{\mathrm{a}} + \varepsilon P_0 H_1 P_0 \quad (3.3)$$

for the adiabatic operator as an operator on $L^2(B)$. By analogy with Sect. 1, we view

$$(P_0 S^\varepsilon P_0)\psi = \int_{F_x} \phi_0 S^\varepsilon(\phi_0\psi)\, \mathrm{d}g_F$$

as an operator on B via the identification $L^2(B) \cong L^2(B) \otimes \mathrm{span}(\phi_0)$. By the same procedure, projecting the potentials in H_1 amounts to averaging them over the fibres with the weight $|\phi_0|^2$.

4. Massive Quantum Waveguides

The vast literature on quantum waveguides is, in our terminology, concerned with the case of massive waveguides. In this section, we give a detailed derivation of the effects due to the extrinsic geometry of $B \subset \mathbb{R}^{d+k}$. The necessary calculations of the metric g^ε and the bending potential V_{bend} have been performed in all of the works on quantum waveguides for the respective special cases, and by Tolar [27] for the leading order V^0_{bend} in the general case. A generalisation to tubes in Riemannian manifolds is due to Wittich [29].

We then discuss the explicit form of the adiabatic Hamiltonian (1.5), calculating the adiabatic potential and the projection of H_1. In particular, we generalise the concept of a "twisted" waveguide (cf. [6]) to arbitrary dimension and codimension in Sect. 4.4.2. We also examine the role of the differential operator S^ε in H_{a}, which is rarely discussed in the literature, and its relevance for the different energy scales ε^α.

4.1. The Pullback Metric

Let $(x^1,\dots,x^d)$ be local coordinates on B and $\{e_\alpha\}_{\alpha=1}^k$ a local orthonormal frame of M with respect to $g_B^\perp := \delta_{d+k}|_{\mathsf{N}B}$ such that every normal vector $\nu(x) \in \mathsf{N}_x B$ may be written as

$$\nu(x) = n^\alpha e_\alpha(x). \tag{4.1}$$

These bundle coordinates yield local coordinate vector fields

$$\partial_i|_{(x,n)} := \tfrac{\partial}{\partial x^i}, \quad \partial_{d+\alpha}|_{(x,n)} := \tfrac{\partial}{\partial n^\alpha} \tag{4.2}$$

on M for $i \in \{1,\dots,d\}$ and $\alpha \in \{1,\dots,k\}$. The aim is to obtain formulas for the coefficients of the unscaled pullback metric $g = \Phi^*\delta_{d+k}|_{\mathsf{T}M}$ with respect to these coordinate vector fields.

Let $I \subset \mathbb{R}$ be an open neighbourhood of zero, $b : I \to M$, $s \mapsto b(s) = (c(s), v(s))$ be a curve with $b(0) = (x,n)$ and $b'(0) = \xi \in \mathsf{T}_{(x,n)}M$. It then holds that

$$\Phi_*\xi = \tfrac{\mathrm{d}}{\mathrm{d}s}\big|_{s=0}\, \Phi\big(b(s)\big) = c'(0) + v'(0).$$

For the case $\xi = \partial_i|_{(x,n)}$, we choose the curve $b : I \to M$ given by

$$b(s) = \Big(c(s), n^\alpha e_\alpha\big(c(s)\big)\Big) \quad \Rightarrow \quad \Phi\big(b(s)\big) = c(s) + n^\alpha e_\alpha\big(c(s)\big)$$

where $c : I \to B$ is a smooth curve with $c(0) = x$ and $c'(0) = \partial_{x^i} \in \mathsf{T}_x B$. We then have

$$\Phi_*\partial_i|_{(x,n)} = c'(0) + n^\alpha\ \tfrac{\mathrm{d}}{\mathrm{d}s}\big|_{s=0}\, e_\alpha\big(c(s)\big) = \partial_{x^i} + n^\alpha \nabla^{\mathbb{R}^{d+k}}_{\partial_{x^i}} e_\alpha(x)$$

To relate the appearing derivative $\nabla^{\mathbb{R}^{d+k}}_{\partial_{x^i}} e_\alpha(x)$ to the extrinsic curvature of B, we project the latter onto its tangent and normal component, respectively. Therefore, we introduce the Weingarten map

$$\mathcal{W} : \Gamma(\mathsf{N}B) \to \mathcal{T}^1_1(B), \quad e_\alpha \mapsto \mathcal{W}(e_\alpha)\partial_{x^i} := -\,\mathrm{P}^{\mathsf{T}B}\, \nabla^{\mathbb{R}^{d+k}}_{\partial_{x^i}} e_\alpha,$$

and the $\mathfrak{so}(k)$-valued local connection one-form associated with the normal connection ∇^{N} with respect to $\{e_\alpha\}_{k=1}^{\alpha}$, i.e.

$$\omega^{\mathsf{N}}(\partial_{x^i})e_\alpha = \nabla^{\mathsf{N}}_{\partial_{x^i}} e_\alpha := \mathrm{P}^{\mathsf{N}B}\, \nabla^{\mathbb{R}^{d+k}}_{\partial_{x^i}} e_\alpha.$$

With these objects, we have

$$\Phi_*\partial_i|_{(x,n)} = \partial_{x^i} + n^\alpha\Big(-\mathcal{W}\big(e_\alpha(x)\big)\partial_{x^i} + \omega^{\mathsf{N}}(\partial_{x^i})e_\alpha(x)\Big). \tag{4.3}$$

For the case $\xi = \partial_{d+\alpha}|_{(x,n)}$, one takes the curve $b : I \to M$ with

$$b(s) = \big(x, \nu(x) + se_\alpha(x)\big) \quad \Rightarrow \quad \Phi\big(b(s)\big) = x + (n^\beta + s\delta_\alpha{}^\beta)e_\beta(x).$$

Hence,

$$\Phi_*\partial_{d+\alpha}|_{(x,n)} = 0 + \tfrac{\mathrm{d}}{\mathrm{d}s}\big|_{s=0}\,(n^\beta + s\delta_\alpha{}^\beta)e_\beta(x) = \delta_\alpha{}^\beta e_\beta(x) = e_\alpha(x). \tag{4.4}$$

Combining the expressions for the tangent maps, we finally obtain the following expressions for the pullback metric g:

Lemma 4.1. *Let (x, n) be the local bundle coordinates on M introduced in (4.1) and (4.2) the associated coordinate vector fields. Then, the coefficients of the pullback metric are given by*

$$\begin{aligned} g_{ij}(x,n) &= g_B(\partial_{x^i},\partial_{x^j}) - 2\,\mathrm{II}(\nu)(\partial_{x^i},\partial_{x^j}) + g_B\big(\mathcal{W}(\nu)\partial_{x^i},\mathcal{W}(\nu)\partial_{x^j}\big)\\ &\quad + g_B^{\perp}\big(\omega^{\mathsf{N}}(\partial_{x^i})\nu, \omega^{\mathsf{N}}(\partial_{x^j})\nu\big),\\ g_{i,d+\alpha}(x,n) &= g_B^{\perp}\big(\omega^{\mathsf{N}}(\partial_{x^i})\nu, e_\alpha\big),\\ g_{d+\alpha,d+\beta}(x,n) &= g_B^{\perp}\big(e_\alpha, e_\beta\big) = \delta_{\alpha\beta} \end{aligned}$$

for $i, j \in \{1, \ldots, d\}$ and $\alpha, \beta \in \{1, \ldots, k\}$. Here, $\mathrm{II} : \Gamma(\mathsf{N}B) \to \mathcal{T}^0_2(B)$ denotes the second fundamental form defined by $\mathrm{II}(\nu)(\partial_{x^i},\partial_{x^j}) := g_B(\mathcal{W}(\nu)\partial_{x^i},\partial_{x^j})$.

Let us now consider the scaled pullback metric $g^\varepsilon = \varepsilon^{-2}\mathcal{D}_\varepsilon^*\Phi^*\delta_{d+k}|_{\mathsf{T}M}$. Observe that for any $\xi \in \mathsf{T}_{(x,n)}M$

$$\begin{aligned} \Phi_*(\mathcal{D}_\varepsilon)_*\xi &= (\Phi\circ\mathcal{D}_\varepsilon)_*\xi\\ &= \tfrac{\mathrm{d}}{\mathrm{d}s}\big|_{s=0}\,(\Phi\circ\mathcal{D}_\varepsilon)\big(b(s)\big) = \tfrac{\mathrm{d}}{\mathrm{d}s}\big|_{s=0}\,(\Phi\circ\mathcal{D}_\varepsilon)\big(c(s), v(s)\big)\\ &= \tfrac{\mathrm{d}}{\mathrm{d}s}\big|_{s=0}\,\Phi\big(c(s), \varepsilon v(s)\big) = c'(0) + \varepsilon v'(0) \end{aligned}$$

and one immediately concludes from (4.3) and (4.4) that

$$\begin{aligned} \Phi_*(\mathcal{D}_\varepsilon)_*\partial_i|_{(x,n)} &= \partial_{x^i} + \varepsilon n_\alpha\Big(-\mathcal{W}\big(e_\alpha(x)\big)\partial_{x^i} + \omega^N(\partial_{x^i})e_\alpha(x)\Big),\\ \Phi_*(\mathcal{D}_\varepsilon)_*\partial_\alpha|_{(x,n)} &= \varepsilon e_\alpha(x). \end{aligned}$$

Consequently, the coefficients of the scaled pullback metric are given by

$$\begin{aligned} g^\varepsilon_{ij}(x,n) &= \varepsilon^{-2}\big[g_B(\partial_{x^i},\partial_{x^j}) - \varepsilon 2\,\mathrm{II}(\nu)(\partial_{x^i},\partial_{x^j})\\ &\quad +\varepsilon^2 g_B\big(\mathcal{W}(\nu)\partial_{x^i},\mathcal{W}(\nu)\partial_{x^j}\big)\\ &\quad +\varepsilon^2 g_B^{\perp}\big(\omega^{\mathsf{N}}(\partial_{x^i})\nu, \omega^{\mathsf{N}}(\partial_{x^j})\nu\big)\big],\\ g^\varepsilon_{i,d+\alpha}(x,n) &= g_B^{\perp}\big(\omega^{\mathsf{N}}(\partial_{x^i})\nu, e_\alpha\big),\\ g^\varepsilon_{d+\alpha,d+\beta}(x,n) &= \delta_{\alpha\beta} \end{aligned}$$

for $i, j \in \{1, \ldots, d\}$ and $\alpha, \beta \in \{1, \ldots, k\}$.

Clearly $\operatorname{span}\{\partial_i|_{(x,n)}\}_{i=1}^d$ is not orthogonal to $\operatorname{span}\{\partial_{d+\alpha}|_{(x,n)}\}_{\alpha=1}^k = \mathsf{V}_{(x,n)}M$ with respect to g^ε. However, any vector $\partial_i|_{(x,n)}$ can be orthogonalised by subtracting its vertical component. The resulting vector

$$\begin{aligned}\partial_{x^i}^{\mathsf{H}M}|_{(x,n)} &:= \partial_i|_{(x,n)} - g^\varepsilon_{i,d+\beta}(x,n)\,\partial_{d+\beta}|_{(x,n)}\\ &= \partial_i|_{(x,n)} - g_B^\perp\big(\omega^{\mathsf{N}}(\partial_{x^i})\nu, e_\beta\big)\,\partial_{d+\beta}|_{(x,n)}\\ &= \partial_i|_{(x,n)} - g_{i,d+\beta}(x,n)\,\partial_{d+\beta}|_{(x,n)} \end{aligned}\tag{4.5}$$

is the horizontal lift of ∂_{x^i}. Consequently, the orthogonal complement of $\mathsf{V}_{(x,n)}M$ with respect to g^ε is given by $\mathsf{H}_{(x,n)}M = \operatorname{span}\{\partial_{x^i}^{\mathsf{H}M}|_{(x,n)}\}_{i=1}^d$ for all $\varepsilon > 0$. Finally, a short computation shows that

$$\begin{aligned}&g^\varepsilon(\partial_{x^i}^{\mathsf{H}M}|_{(x,n)}, \partial_{x^j}^{\mathsf{H}M}|_{(x,n)})\\ &= \varepsilon^{-2} g_B\Big(\big(1-\varepsilon\mathcal{W}(\nu)\big)\partial_{x^i}, \big(1-\varepsilon\mathcal{W}(\nu)\big)\partial_{x^j}\Big)\\ &= \varepsilon^{-2}\Big[g_B(\partial_{x^i},\partial_{x^j}) + \varepsilon\Big(-2\,\mathrm{II}(\nu)(\partial_{x^i},\partial_{x^j}) + \varepsilon g_B\big(\mathcal{W}(\nu)\partial_{x^i}, \mathcal{W}(\nu)\partial_{x^j}\big)\Big)\Big].\end{aligned}\tag{4.6}$$

Hence, the scaled pullback metric g^ε actually has the form (2.2) with "horizontal correction"

$$h^\varepsilon(\partial_{x^i}^{\mathsf{H}M}|_{(x,n)}, \partial_{x^j}^{\mathsf{H}M}|_{(x,n)}) = -2\,\mathrm{II}(\nu)(\partial_{x^i},\partial_{x^j}) + \varepsilon g_B\big(\mathcal{W}(\nu)\partial_{x^i}, \mathcal{W}(\nu)\partial_{x^j}\big).\tag{4.7}$$

Remark 4.2. The fibres F_x of M are completely geodesic for the pullback metric g^ε. To see this, we show that the second fundamental form of the fibres $\mathrm{II}^F|_x : \mathsf{H}_xM \to \mathcal{T}_2^0(F_x)$ vanishes identically. Since the latter is a symmetric tensor, it is sufficient to show that the diagonal elements

$$\mathrm{II}^F(\partial_{x^i}^{\mathsf{H}M})(\partial_\alpha,\partial_\alpha) = g^\varepsilon(\nabla^M_{\partial_\alpha}\partial_\alpha, \partial_{x^i}^{\mathsf{H}M})$$

are zero. Using Koszul's formula, four out of the six appearing terms obviously vanish and we are left with

$$\begin{aligned}\mathrm{II}^F(\partial_{x^i}^{\mathsf{H}M})(\partial_\alpha,\partial_\alpha) &= g_F\left([\partial_{x^i}^{\mathsf{H}M},\partial_\alpha],\partial_\alpha\right)\\ &\overset{(4.5)}{=} g_F\Big(\underbrace{[\partial_i,\partial_\alpha]}_{=0} - \big[g_{i,d+\beta}(x,n)\partial_\beta,\partial_\alpha\big],\partial_\alpha\Big)\\ &= \frac{g_{i,d+\beta}(x,n)}{\partial n^\alpha}\underbrace{g_F(\partial_\beta,\partial_\alpha)}_{\delta_{\beta\alpha}}\\ &= g_B^\perp(\omega^{\mathsf{N}}(\partial_{x^i})e_\alpha, e_\alpha).\end{aligned}$$

But now, the last expression equals zero since $\omega^{\mathsf{N}}(\partial_{x^i})$ is $\mathfrak{so}(k)$-valued. Consequently, the mean curvature vector η_F defined by

$$\mathrm{tr}_{\mathsf{T}F}\,\mathrm{II}(\partial_{x^i}^{\mathsf{H}M}) = \pi_M^* g_B(\partial_{x^i}^{\mathsf{H}M}, \eta_F)\tag{4.8}$$

vanishes identically. Finally note that the same considerations also hold for the submersion metric $g_{\mathrm{s}}^\varepsilon$ due to $g^\varepsilon|_{\mathsf{V}M} = g_F = g_{\mathrm{s}}^\varepsilon|_{\mathsf{V}M}$.

4.2. The Horizontal Laplacian

Now that we have a detailed description of the metric, we can explicitly express the horizontal Laplacian by the vector fields $(\{\partial^{\mathsf{H}M}_{x^i}\}_{i=1}^d, \{\partial_{d+\alpha}\}_{\alpha=1}^k)$. Let $(\{\pi_M^* \mathrm{d}x^i\}_{i=1}^d, \{\delta n^\alpha\}_{\alpha=1}^k)$ be the dual basis (note that in general $\delta n^\alpha \neq \mathrm{d}n^\alpha$ since $\mathrm{d}n^\alpha(\partial^{\mathsf{H}M}_{x^i}) \neq 0$). Then by definition

$$\begin{aligned}\delta n^\alpha(\mathrm{P}^{\mathsf{H}M} \operatorname{grad}_{g_\mathrm{s}} \psi) &= 0,\\ \pi_M^* \mathrm{d}x^i(\mathrm{P}^{\mathsf{H}M} \operatorname{grad}_{g_\mathrm{s}} \psi) &= g_\mathrm{s}^{jk}(\partial^{\mathsf{H}M}_{x^j}\psi)\mathrm{d}x^i(\partial_{x^k}) = g_B^{ij}\partial^{\mathsf{H}M}_{x^j}\psi\end{aligned}$$

and thus

$$\operatorname{grad}_{g_\mathrm{s}} \psi = g_B^{ij}(\partial^{\mathsf{H}M}_{x^i}\psi)\partial^{\mathsf{H}M}_{x^j}.$$

When acting on a horizontal vector field Y, the divergence takes the coordinate form

$$\begin{aligned}\operatorname{div}_{g_\mathrm{s}} Y &= \frac{1}{\sqrt{|g_\mathrm{s}|}}\partial^{\mathsf{H}M}_{x^i}\sqrt{|g_\mathrm{s}|}(\pi_M^*\mathrm{d}x^i(Y))\\ &= \frac{1}{\sqrt{|g_B|}}\partial^{\mathsf{H}M}_{x^i}\sqrt{|g_B|}\big(\pi_M^*\mathrm{d}x^i(Y)\big) - \pi_M^* g_B(\eta_F, Y), \qquad (4.9)\end{aligned}$$

since $\sqrt{|g_F|}^{-1}\big(\partial^{\mathsf{H}M}_{x^i}\sqrt{|g_F|}\big) = -g_\mathrm{s}(\eta_F, \partial^{\mathsf{H}M}_{x^i})$. For a horizontal lift $X^{\mathsf{H}M}$, we have the simple formula

$$\operatorname{div}_{g_\mathrm{s}} X^{\mathsf{H}M} = \pi_M^*\big(\operatorname{div}_{g_B} X - g_B(\pi_{M*}\eta_F, X)\big).$$

Now for a massive waveguide $\eta_F = 0$ and the horizontal Laplacian takes the familiar form

$$\Delta_\mathsf{H} = \frac{1}{\sqrt{|g_B|}}\partial^{\mathsf{H}M}_{x^i}\sqrt{|g_B|}g_B^{ij}\partial^{\mathsf{H}M}_{x^j},$$

which is just Δ_{g_B} with ∂_{x^i} replaced by $\partial^{\mathsf{H}M}_{x^i}$.

4.3. The Bending Potential

In Sect. 1 [see Eq. (1.4)], we saw that the leading order of V_bend is attractive (negative) and proportional to the square of the curve's curvature $\kappa = |c''|$. Here, we give a detailed derivation of V_bend for generalised massive waveguides and then discuss the sign of its leading part. Therefore, let $\{\tau_i\}_{i=1}^d$ be a local orthonormal frame of $\mathsf{T}B$ with respect to g_B and let $\{n^\alpha\}_{\alpha=1}^k$ be coordinates on $\mathsf{N}B$ as in Eq. (4.1). Then

$$T_i := \tau_i^{\mathsf{H}M}, \quad N_\alpha := \tfrac{\partial}{\partial n^\alpha}$$

for $i \in \{1, \ldots, d\}$ and $\alpha \in \{1, \ldots, k\}$ form a local frame of $\mathsf{T}M$. In this frame, the scaled metrics have the form [see also (4.6)]

$$g^\varepsilon = \left(\begin{array}{c|c}\varepsilon^{-2}(\mathrm{id}_{d\times d} - \varepsilon\mathcal{W}(\nu))^2 & 0\\ \hline 0 & \mathrm{id}_{k\times k}\end{array}\right), \quad g_\mathrm{s}^\varepsilon = \left(\begin{array}{c|c}\varepsilon^{-2}\,\mathrm{id}_{d\times d} & 0\\ \hline 0 & \mathrm{id}_{k\times k}\end{array}\right).$$

From that and Eq. (2.3), we easily conclude that

$$\rho_\varepsilon = \sqrt{\frac{\det(g^\varepsilon)}{\det(g_\mathrm{s}^\varepsilon)}} = \det\big(\mathrm{id}_{d\times d} - \varepsilon\mathcal{W}(\nu)\big) = \exp\Big(\operatorname{tr}\log\big(\mathrm{id}_{d\times d} - \varepsilon\mathcal{W}(\nu)\big)\Big).$$

Using Taylor's expansion for ε small enough

$$-\log\big(\mathrm{id}_{d\times d} - \varepsilon\mathcal{W}(\nu)\big) = \underbrace{\varepsilon\mathcal{W}(\nu) + \tfrac{\varepsilon^2}{2}\mathcal{W}(\nu)^2 + \tfrac{\varepsilon^3}{3}\mathcal{W}(\nu)^3}_{=:\mathcal{Z}(\varepsilon)} + \mathcal{O}(\varepsilon^4),$$

we have $\log(\rho_\varepsilon) = -\operatorname{tr}\mathcal{Z}(\varepsilon) + \mathcal{O}(\varepsilon^4)$. Next, we calculate the terms appearing in V_{bend} (2.5) separately:

$$\begin{aligned}
\Delta_{\mathsf{H}} \log\rho_\varepsilon &= -\varepsilon\Delta_{\mathsf{H}} \operatorname{tr}\mathcal{W}(\nu) + \mathcal{O}(\varepsilon^2),\\
\varepsilon^{-2}\Delta_{\mathsf{V}} \log\rho_\varepsilon &= -\varepsilon^{-2}\sum_{\alpha=1}^{k} \partial^2_{n^\alpha} \operatorname{tr}\mathcal{Z}(\varepsilon) + \mathcal{O}(\varepsilon^2)\\
&= -\sum_{\alpha=1}^{k}\Big[\operatorname{tr}\big(\mathcal{W}(e_\alpha)^2\big) + 2\varepsilon\operatorname{tr}\big(\mathcal{W}(e_\alpha)^2\mathcal{W}(\nu)\big)\Big] + \mathcal{O}(\varepsilon^2),\\
\mathrm{d}\log\rho_\varepsilon &= \mathrm{P}^{\mathsf{H}M}\,\mathrm{d}\log\rho_\varepsilon - \operatorname{tr}\big(\partial_{n_\alpha}\mathcal{Z}(\varepsilon)\big)\,\mathrm{d}n^\alpha + \mathcal{O}(\varepsilon^4)\\
&= \mathrm{P}^{\mathsf{H}M}\,\mathrm{d}\log\rho_\varepsilon - \operatorname{tr}\Big(\varepsilon\mathcal{W}(e_\alpha)\big(\mathrm{id}_{d\times d} + \varepsilon\mathcal{W}(\nu) + \varepsilon^2\mathcal{W}(\nu)^2\big)\Big)\,\mathrm{d}n^\alpha\\
&\quad + \mathcal{O}(\varepsilon^4),
\end{aligned}$$

denoting by $\mathrm{P}^{\mathsf{H}M}$ the adjoint of the original $\mathrm{P}^{\mathsf{H}M}$ with respect to the pairing of T^*M and $\mathsf{T}M$, and hence

$$\begin{aligned}
&\varepsilon^{-2} g_F(\mathrm{d}\log\rho_\varepsilon, \mathrm{d}\log\rho_\varepsilon)\\
&\quad = \sum_{\alpha=1}^{k}\Big[\big(\operatorname{tr}\mathcal{W}(e_\alpha)\big)^2 + 2\varepsilon\operatorname{tr}\big(\mathcal{W}(e_\alpha)\big)\operatorname{tr}\big(\mathcal{W}(e_\alpha)\mathcal{W}(\nu)\big)\Big] + \mathcal{O}(\varepsilon^2).
\end{aligned}$$

Putting all this together, we obtain the following expression for the bending potential in the case of massive quantum waveguides:

$$\begin{aligned}
V_{\mathrm{bend}} &= \frac{1}{4}\sum_{\alpha=1}^{k}\Big[\big(\operatorname{tr}\mathcal{W}(e_\alpha)\big)^2 - 2\operatorname{tr}\big(\mathcal{W}(e_\alpha)^2\big)\Big] && (4.10)\\
&= +\frac{\varepsilon}{2}\sum_{\alpha=1}^{k}\Big[\operatorname{tr}\mathcal{W}(e_\alpha)\operatorname{tr}\big(\mathcal{W}(e_\alpha)\mathcal{W}(\nu)\big) - 2\operatorname{tr}\big(\mathcal{W}(e_\alpha)^2\mathcal{W}(\nu)\big)\\
&\qquad - \Delta_{\mathsf{H}}\operatorname{tr}\mathcal{W}(\nu)\Big] && (4.11)\\
&= +\mathcal{O}(\varepsilon^2).
\end{aligned}$$

The leading term of this expression ($V^0_{\mathrm{bend}} := (4.10)$) has been widely stressed in the literature concerning one-dimensional quantum waveguides (see e.g. [5, 6, 10]), where it has a purely attractive effect. Its higher dimensional versions were discussed by Tolar [27] but are generally less known, so we will discuss their possible effects for the rest of this section.

Since $\mathcal{W}(e_\alpha)$ is self-adjoint, we may choose for each $\alpha \in \{1, \ldots, k\}$ the orthonormal frame $\{\tau_i\}_{i=1}^d$ such that it consists of the eigenvectors of $\mathcal{W}(e_\alpha)$ with eigenvalues (principal curvatures) $\{\kappa_i^\alpha\}_{i=1}^d$. To get an impression of V^0_{bend}'s sign, we divide $\mathcal{W}(e_\alpha)$ into a traceless part $\mathcal{W}_0(e_\alpha)$ and a multiple of the identity:

$$\mathcal{W}(e_\alpha) = \mathcal{W}_0(e_\alpha) + \frac{H_\alpha}{d}\,\mathrm{id}_{d\times d}\,.$$

Note that the prefactors H_α equal the components of the mean curvature vector of B in direction e_α. With the notation

$$\|M\|^2 := \mathrm{tr}\big(M^{\mathrm{t}}M\big) \geq 0$$

for any $M \in \mathbb{R}^{d\times d}$, we get the relation

$$\|\mathcal{W}(e_\alpha)\|^2 = \|\mathcal{W}_0(e_\alpha)\|^2 + \frac{H_\alpha^2}{d}$$

for all $\alpha \in \{1,\dots,k\}$ since $\mathcal{W}_0(\cdot)$ is traceless. This yields for the potential (4.10):

$$\begin{aligned} V^0_{\mathrm{bend}} &= \frac{1}{4}\sum_{\alpha=1}^{k}\big[H_\alpha^2 - 2\,\|\mathcal{W}(e_\alpha)\|^2\big] \\ &= \frac{1}{4}\sum_{\alpha=1}^{k}\left[H_\alpha^2 - 2\left(\|\mathcal{W}_0(e_\alpha)\|^2 + \frac{H_\alpha^2}{d}\right)\right] \\ &= \frac{1}{4}\sum_{\alpha=1}^{k}\left[\left(1-\frac{2}{d}\right)H_\alpha^2 - 2\,\|\mathcal{W}_0(e_\alpha)\|^2\right]. \end{aligned}$$

The latter relation shows that for $d \in \{1,2\}$ the leading order of the bending potential is non-positive. Thus, the effect of bending has an attractive character ($V^0_{\mathrm{bend}} < 0$) for ε small enough, or is of lower order ($V^0_{\mathrm{bend}} = 0$), independently of the codimension k. For $d \geq 3$, the first term is non-negative and may overcompensate the second term leading to a positive contribution to V_{bend}. Consequently, a repulsive bending effect is possible.

Example. We may rewrite expression (4.10) in terms of principal curvatures as:

$$V^0_{\mathrm{bend}} = \frac{1}{4}\sum_{\alpha=1}^{k}\left[\left(\sum_{i=1}^{d}\kappa_i^\alpha\right)^2 - 2\sum_{i=1}^{d}(\kappa_i^\alpha)^2\right]. \tag{4.12}$$

(a) For a waveguide modelled around a curve c, $d = 1$, one immediately sees that $V^0_{\mathrm{bend}} = -\frac{1}{4}\kappa^2 = -\frac{1}{4}\,|c''|^2$.

(b) We consider the case where $B \subset \mathbb{R}^{d+1}$ is the d-dimensional standard sphere of radius R. The principal curvatures in the direction of the outer-pointing normal are given by $\kappa_i = 1/R$ for all $i \in \{1,\dots,d\}$, hence the bending potential (4.12) reads

$$V^0_{\mathrm{bend}} = \frac{1}{4}\left[\left(\sum_{i=1}^{d}\frac{1}{R}\right)^2 - 2\sum_{i=1}^{d}\left(\frac{1}{R}\right)^2\right] = \left(1-\frac{2}{d}\right)\frac{d^2}{4R^2}.$$

It follows that $V^0_{\mathrm{bend}} < 0$ for $d = 1$, $V^0_{\mathrm{bend}} = 0$ for $d = 2$ and $V^0_{\mathrm{bend}} > 0$ for $d \geq 3$, respectively. Thus, depending on the dimension d of the sphere, the effect of bending can be either attractive or repulsive.

4.4. The Adiabatic Hamiltonian

We are now ready to calculate the geometric terms in the adiabatic operator. In this, we concentrate on the adiabatic operator (3.3) and explicitly calculate all the relevant terms on the energy scale given by Theorem 3.3. First, we take care of the contribution of H_1, then we turn to the potential V_{a} and explain its connection to "twisting" of the quantum waveguide.

4.4.1. The Operator $P_0 H_1 P_0$. The contribution of the bending potential, that was calculated in the previous section, is given by its adiabatic approximation

$$V^{\mathrm{a}}_{\mathrm{bend}} := P_0 V_{\mathrm{bend}} P_0 = \int_{F_x} V_{\mathrm{bend}}(\nu)\,|\phi_0(\nu)|^2\,\mathrm{d}\nu.$$

Since the leading part V^0_{bend} is independent of the fibre coordinate ν, it is unchanged by this projection. The next term in the expansion of V_{bend} is given by (4.11). The Weingarten map is linear in ν and since

$$\partial^{\mathsf{H}M}_{x^i} n^\alpha \overset{(4.5)}{=} -g^\perp_B\big(\omega^{\mathsf{N}}(\partial_{x^i})\nu, e_\beta\big)\partial_{n^\beta} n^\alpha = -g^\perp_B\big(\omega^{\mathsf{N}}(\partial_{x^i})\nu, e_\alpha\big)$$

is again linear in ν, $\Delta_{\mathsf{H}}\,\mathrm{tr}\,\mathcal{W}(\nu)$ is also linear in ν. Consequently, the contribution of (4.11) to $V^{\mathrm{a}}_{\mathrm{bend}}$ is proportional to

$$\langle\phi_0, \nu\phi_0\rangle_{L^2(F_x)} = \int_{F_x} \nu\,|\phi_0(\nu)|^2\,\mathrm{d}\nu.$$

Hence, this contribution vanishes if the centre of mass of the ground state ϕ_0 lies exactly on the submanifold B. This is a reasonable assumption to make and represents a "correct" choice of parametrisation of the waveguide. Under this assumption, we have

$$V^{\mathrm{a}}_{\mathrm{bend}} = V^0_{\mathrm{bend}} + \mathcal{O}(\varepsilon^2).$$

From the expression (4.6) for the horizontal block of the metric g^ε, one obtains its expansion on horizontal one-forms by locally inverting the matrix $(g^\varepsilon)_{ij}$ (see [29]). The result is

$$g^\varepsilon(\pi^*_M \mathrm{d}x^i, \pi^*_M \mathrm{d}x^j) = \varepsilon^2\big(g^{ij}_B + 2\varepsilon\,\mathrm{II}(\nu)^{ij} + \mathcal{O}(\varepsilon^2)\big), \tag{4.13}$$

where II denotes the second fundamental form of B, defined on T^*B by $\mathrm{II}^{ij} := \mathrm{II}_{kl}\, g^{ik}_B g^{jl}_B$. Moreover, we extend the latter to T^*M, understanding $\mathrm{II}(\nu)$ as its lift to the horizontal part H^*M and extending to T^*M by zero. The vertical components of g^ε and $g^\varepsilon_{\mathrm{s}}$ coincide, hence as an operator on $L^2(B)$ we have the expression

$$(P_0 S^\varepsilon P_0)\psi = 2\int_{F_x} \phi_0\,\mathrm{div}_{g_{\mathrm{s}}}\Big(\mathrm{II}(\nu)\big(\mathrm{d}(\phi_0\psi),\cdot\big)\Big)\,\mathrm{d}\nu + \mathcal{O}(\varepsilon) \tag{4.14}$$

with an error of order ε on $W^2(B)$. Using the Leibniz rule, we can rewrite this as:

$$\begin{aligned}2\int_{F_x} & 2\phi_0\,\mathrm{II}(\nu)\big(\mathrm{d}\phi_0,\mathrm{d}\psi\big)+|\phi_0|^2\,\mathrm{div}_{g_\mathrm{s}}\big(\mathrm{II}(\nu)(\mathrm{d}\psi,\cdot)\big)\\ &+\phi_0\psi\,\mathrm{div}_{g_\mathrm{s}}\big(\mathrm{II}(\nu)(\mathrm{d}\phi_0,\cdot)\big)\mathrm{d}\nu\\ &=2\int_{F_x}\mathrm{div}_{g_\mathrm{s}}\big(|\phi_0|^2\,\mathrm{II}(\nu)(\mathrm{d}\psi,\cdot)\big)+\phi_0\psi\,\mathrm{div}_{g_\mathrm{s}}\big(\mathrm{II}(\nu)(\mathrm{d}\phi_0,\cdot)\big)\mathrm{d}\nu. \quad (4.15)\end{aligned}$$

Now ϕ_0 vanishes on the boundary and $\mathrm{II}(\mathrm{d}\psi,\cdot)$ is a horizontal vector field, so by (4.9) we have

$$\int_{F_x}\mathrm{div}_{g_\mathrm{s}}\big(|\phi_0|^2\,\mathrm{II}(\nu)(\mathrm{d}\psi,\cdot)\big)\mathrm{d}\nu=\mathrm{div}_{g_B}\int_{F_x}|\phi_0|^2\,\mathrm{II}(\nu)(\mathrm{d}\psi,\cdot)\mathrm{d}\nu. \quad (4.16)$$

If we assume again that ϕ_0 is centred on B, this term vanishes and we are left with the potential

$$\varepsilon P_0H_1P_0=\varepsilon^2V^0_{\mathrm{bend}}-2\varepsilon^3\int_{F_x}\phi_0\,\mathrm{div}_{g_\mathrm{s}}\big(\mathrm{II}(\nu)(\mathrm{d}\phi_0,\cdot)\big)\mathrm{d}\nu+\mathcal{O}(\varepsilon^4) \quad (4.17)$$

with an error bound in $\mathcal{L}\big(W^2(B),L^2(B)\big)$.

4.4.2. The Adiabatic Potential V_a and "Twisted" Waveguides. Since the fibres F_x are completely geodesic with respect to g_F for massive quantum waveguides (cf. Remark 4.2), we have $\eta_F=0$ and the adiabatic potential defined in (3.2) reduces to

$$V_\mathrm{a}=\int_{F_x}\pi^*_M g_B(\mathrm{grad}_{g_\mathrm{s}}\phi_0,\mathrm{grad}_{g_\mathrm{s}}\phi_0)\mathrm{d}\nu. \quad (4.18)$$

This is called the Born–Huang potential in the context of the Born–Oppenheimer approximation. This potential is always non-negative. It basically accounts for the alteration rate of ϕ_0 in horizontal directions.

In the literature, the adiabatic potential has been studied mainly for "twisted" quantum waveguides. These have two-dimensional fibres F_x which are isometric but not invariant under rotations and twist as one moves along the one-dimensional base curve B [6]. The operators Δ_{F_x}, $x\in B$, are isospectral and their non-trivial dependence on x is captured by V_a.

We now generalise this concept to massive waveguides of arbitrary dimension and codimension and calculate the adiabatic potential for this class of examples. In this context, a massive quantum waveguide $F\to M\xrightarrow{\pi_M}B$ is said to be only twisted at $x_0\in B$, if there exist a geodesic ball $U\subset B$ around x_0 and a local orthonormal frame $\{f_\alpha\}_{\alpha=1}^k$ of $\mathsf{N}B|_U$ such that

$$\pi_M^{-1}(U)=\big\{n^\alpha f_\alpha(x):\ (n^1,\dots,n^k)\in F,\ x\in U\big\}.$$

This exactly describes the situation that the cross sections (F_x,g_{F_x}) are isometric to $F\subset\mathbb{R}^k$, but may vary from fibre to fibre by an $\mathrm{SO}(k)$-transformation. Moreover, it follows that λ_0 is constant on U and the associated eigenfunction ϕ_0 is of the form $\phi_0(\nu(x)=n^\alpha f_\alpha(x))=\Phi_0(n^1,\dots,n^k)$, where Φ_0 is the solution of

$$-\Delta_n\Phi_0(n)=\lambda_0\Phi_0(n),\quad \Phi_0(n)=0\quad \text{on }\partial F.$$

As for the calculation of V_{a} at x_0, we firstly compute for $\partial_{x^i}^{\mathsf{H}M} \in \Gamma(\mathsf{H}M)$:

$$\begin{aligned}\pi_M^* g_B(\operatorname{grad}_{g_{\mathrm{s}}} \phi_0, \partial_{x^i}^{\mathsf{H}M})|_{\nu(x_0)} &= g_{\mathrm{s}}(\operatorname{grad}_{g_{\mathrm{s}}} \phi_0, \partial_{x^i}^{\mathsf{H}M})|_{\nu(x_0)} \\ &= \partial_{x^i}^{\mathsf{H}M} \phi_0\big|_{\nu(x_0)} \\ &\overset{(4.5)}{=} \Big[\partial_i - g_B^{\perp}\big(\omega^{\mathsf{N}}(\partial_{x^i})\nu, f_\beta\big)\big|_{x_0} \partial_{n^\beta}\Big] \Phi_0(n) \\ &= -n^\alpha g_B^{\perp}\big(\nabla^{\mathsf{N}}_{\partial_{x^i}} f_\alpha, f_\beta\big)\big|_{x_0} \frac{\partial \Phi_0(n)}{\partial n^\beta}. \end{aligned} \tag{4.19}$$

To get a better understanding of $g_B^{\perp}(\nabla^{\mathsf{N}}_{\partial_{x^i}} f_\alpha, f_\beta)|_{x_0}$, we introduce on U a locally untwisted orthonormal frame $\{e_\alpha\}_{\alpha=1}^k$ of $\mathsf{N}B|_U$. It is obtained by taking the vectors $f_\alpha(x_0) \in \mathsf{N}_{x_0}B$ and parallel transporting them along radial geodesics with respect to the normal connection ∇^{N}. Thus, twisting is always to be understood relative to the locally parallel frame $\{e_\alpha\}_{\alpha=1}^k$. The induced map that transfers the reference frame $\{e_\alpha\}_{\alpha=1}^k$ into the twisting frame $\{f_\alpha\}_{\alpha=1}^k$ is denoted by $R : U \to \mathrm{SO}(k)$. It is defined by the relation $f_\alpha(x) = e_\gamma(x) R^\gamma{}_\alpha(x)$ for $x \in U$ and obeys $R(x_0) = \mathrm{id}_{k\times k}$ due to the initial data of $\{e_\alpha\}_{\alpha=1}^k$. Consequently, using the differential equation of the parallel transport, we have

$$\nabla^{\mathsf{N}}_{\partial_{x^i}} f_\alpha(x_0) = \nabla^{\mathsf{N}}_{\partial_{x^i}} (e_\gamma R^\gamma{}_\alpha)(x_0) = \underbrace{\big(\nabla^{\mathsf{N}}_{\partial_{x^i}} e_\gamma\big)(x_0)}_{=0} \delta^\gamma{}_\alpha + e_\gamma(x)\, \partial_{x^i} R^\gamma{}_\alpha(x_0)$$

and hence

$$g_B^{\perp}\big(\nabla^{\mathsf{N}}_{\partial_{x^i}} f_\alpha, f_\beta\big)\big|_{x_0} = g_B^{\perp}(e_\gamma\, \partial_{x^i} R^\gamma{}_\alpha, e_\beta)|_{x_0} = \partial_{x^i} R_{\beta\alpha}(x_0). \tag{4.20}$$

For $1 \le \alpha < \beta \le k$, let $T_{\alpha\beta} \in \mathbb{R}^{k\times k}$ defined by

$$(T_{\alpha\beta})_{\gamma\zeta} := \delta_{\alpha\zeta}\delta_{\beta\gamma} - \delta_{\alpha\gamma}\delta_{\beta\zeta}$$

be a set of generators of the Lie Algebra $\mathfrak{so}(k)$. This induces generalised angle functions $\{\omega^{\alpha\beta} \in C^\infty(U)\}_{\alpha<\beta}$ by the relation

$$R(x) = \exp\Big(\sum_{\alpha<\beta} \omega^{\alpha\beta}(x) T_{\alpha\beta}\Big)$$

for $x \in U$. Then, a short calculation shows that

$$\partial_{x^i} R(x_0) = \big((\partial_{x^i} \omega^{\alpha\beta} T_{\alpha\beta}) R\big)(x_0) = \mathrm{d}\omega^{\alpha\beta}(\partial_{x^i})|_{x_0} T_{\alpha\beta}, \quad \alpha < \beta. \tag{4.21}$$

Combining (4.19), (4.20) and (4.21), we obtain

$$\pi_M^* g_B(\operatorname{grad}_{g_{\mathrm{s}}} \phi_0, \partial_{x^i}^{\mathsf{H}M})|_{\nu(x_0)=n^\alpha f_\alpha(x_0)} = -\mathrm{d}\omega^{\alpha\beta}(\partial_{x^i})|_{x_0} (L_{\alpha\beta}\Phi_0)(n)$$

for $\alpha < \beta$, where

$$(L_{\alpha\beta}\Phi_0)(n) := \langle (\nabla_n \Phi_0)(n), T_{\alpha\beta} n\rangle_{\mathbb{R}^k} = (n^\alpha \partial_{n^\beta} - n^\beta \partial_{n^\alpha})\Phi_0(n)$$

defines the action of the (α, β)-component of the angular momentum operator in k dimensions. From here, it is easy to see that the adiabatic potential at x_0 is given by

$$
\begin{aligned}
V_{\mathrm{a}}(x_0) &= \int_{F_{x_0}} \pi_M^* g_B(\operatorname{grad}_{g_\mathrm{s}} \phi_0, \operatorname{grad}_{g_\mathrm{s}} \phi_0)\, \mathrm{d}\nu \\
&= \int_F g_B\big(-\mathrm{d}\omega^{\alpha\beta}(L_{\alpha\beta}\Phi_0)(n), -\mathrm{d}\omega^{\gamma\zeta}(L_{\gamma\zeta}\Phi_0)(n)\big)\big|_{x_0}\, \mathrm{d}n \\
&= \underbrace{g_B(\mathrm{d}\omega^{\alpha\beta}, \mathrm{d}\omega^{\gamma\zeta})|_{x_0}}_{=:\mathbf{R}^{(\alpha\beta),(\gamma\zeta)}(x_0)} \underbrace{\langle L_{\alpha\beta}\Phi_0, L_{\gamma\zeta}\Phi_0\rangle_{L^2(F)}}_{=:\mathbf{L}_{(\alpha\beta),(\gamma\zeta)}}, \quad \alpha < \beta \text{ and } \gamma < \zeta \\
&= \operatorname{tr}_{\mathbb{R}^{k(k-1)/2}}\big(\mathbf{R}(x_0)^{\mathrm{t}}\mathbf{L}\big).
\end{aligned} \tag{4.22}
$$

The first matrix $\mathbf{R}(x_0)$ encodes the rate, at which the frame $\{f_\alpha\}_{\alpha=1}^k$ twists relatively to the parallel frame $\{e_\alpha\}_{\alpha=1}^k$ at x_0. The second matrix $\mathbf{L}$ measures the deviation of the eigenfunction Φ_0 from being rotationally invariant. It determines to which extent the twisting of the waveguide effects the states in the range of P_0 and it depends only on the set $F \subset \mathbb{R}^k$ (and not on the point x_0 of the submanifold B). Finally for the case of a twisted quantum waveguides with $(B, g_B) \cong (\mathbb{R}, \delta_1)$ and $k = 2$, there exists only one angle function $\omega \in C^\infty(\mathbb{R})$ and one angular momentum operator $L = n^1\partial_{n^2} - n^2\partial_{n^1}$. Then, formula (4.22) yields the well-known result [14]

$$
V_{\mathrm{a}} = (\omega')^2 \left\|L\Phi_0\right\|_{L^2(F)}^2,
$$

which clearly vanishes if F is invariant under rotations.

4.4.3. Conclusion. Now that we have calculated all the relevant quantities, we can give an explicit expansion of H_{a}. The correct norm for error bounds of course depends on the energy scale under consideration. For a constant eigenvalue λ_0 and $\alpha = 2$ the graph-norm of $\varepsilon^{-2}H_{\mathrm{a}}$ is clearly equivalent (with constants independent of ε) to the usual norm of $W^2(B, g_B)$. In this situation, the best approximation by H_{a} given by Theorem 3.3 has errors of order ε^4, so the estimates just derived give

$$
\begin{aligned}
H_{\mathrm{a}} &= -\varepsilon^2\Delta_{g_B} + \lambda_0 + \varepsilon^2 V_{\mathrm{a}} + \varepsilon^2 V_{\mathrm{bend}}^0 \\
&\quad - 2\varepsilon^3 \int_{F_x} \phi_0 \operatorname{div}_{g_\mathrm{s}}\big(\mathrm{II}(\nu)(\mathrm{d}\phi_0, \cdot)\big)\, \mathrm{d}\nu + \mathcal{O}(\varepsilon^4)
\end{aligned} \qquad (\alpha = 2)
$$

if ϕ_0 is centred. If this is not the case, the expansion can be read off from Eqs. (4.11), (4.14) and (4.18).

If λ_0 has a non-degenerate minimum and $\alpha = 1$, the errors of our best approximation are of order ε^3. Thus, the potentials of order ε^3 can be disregarded in this case. Note, however, that on the domain of $\varepsilon^{-1}H_{\mathrm{a}}$ we have $\varepsilon\partial_{x^i}^{\mathsf{H}M} = \mathcal{O}(\sqrt{\varepsilon})$, so the differential operator (4.16) will be relevant. The error terms of Eq. (4.17), containing second order differential operators, are of order ε^3 with respect to $\varepsilon^{-1}H_{\mathrm{a}}$, so they are still negligible. Thus, for $\psi \in W^2(B)$ with $\|\psi\|^2 + \left\|(-\varepsilon\Delta_{g_B} + \varepsilon^{-1}\lambda_0)\psi\right\|^2 = \mathcal{O}(1)$ we have

$$
\begin{aligned}
H_{\mathrm{a}}\psi &= \big(-\varepsilon^2\Delta_{g_B} + \lambda_0 + \varepsilon^2 V_{\mathrm{a}} + \varepsilon^2 V_{\mathrm{bend}}^0\big)\psi \\
&\quad - 2\varepsilon^3 \operatorname{div}_{g_B} \int_{F_x} |\phi_0(\nu)|^2\, \mathrm{II}(\nu)(\mathrm{d}\psi, \cdot)\, \mathrm{d}\nu + \mathcal{O}(\varepsilon^3),
\end{aligned} \qquad (\alpha = 1)
$$

where the last term is of order ε^2 in general and vanishes for centred ϕ_0.

5. Hollow Quantum Waveguides

In this section, we consider hollow quantum waveguides $F \to (M, g^\varepsilon) \xrightarrow{\pi_M} (B, g_B)$, which by Definition 2.2 are the boundaries of massive waveguides. This underlying massive waveguide is denoted by $\mathring{F} \to (\mathring{M}, \mathring{g}^\varepsilon) \xrightarrow{\pi_{\mathring{M}}} (B, g_B)$ in the following. The bundle structure is inherited from the massive waveguide as well, i.e. $F = \partial\mathring{F}$ and the diagram

$$\begin{array}{ccc} M & \hookrightarrow & \mathring{M} \\ {\scriptstyle \pi_M}\downarrow & & \downarrow{\scriptstyle \pi_{\mathring{M}}} \\ B & \xrightarrow[\mathrm{id}_B]{} & B \end{array}$$

commutes.

Hollow quantum waveguides have, to our knowledge, not been studied before. In fact, already the derivations of g^ε and V_{bend} constitute novel results. A slight generalisation of these calculations to objects that are not necessarily boundaries can be found in [15, Chapter 3].

To determine the adiabatic operator H_{a} for hollow quantum waveguides, we follow the same procedure as layed out in Sect. 1 and in the previous section.

5.1. The Pullback Metric

Note that $g^\varepsilon = \mathring{g}^\varepsilon|_{\mathsf{T}M}$ and that we computed the unscaled pullback metric $\mathring{g}^{\varepsilon=1}$ for the massive waveguide $\mathring{M}$ already in Lemma 4.1. The latter reads

$$\mathring{g} := \mathring{g}^{\varepsilon=1} = \underbrace{\pi^*_{\mathring{M}} g_B + \mathring{h}^{\varepsilon=1}}_{=:\mathring{g}^{\mathrm{hor}}} + g_{\mathring{F}},$$

where the "horizontal correction" $\mathring{h}^{\varepsilon=1}$ (4.7) vanishes on vertical vector fields and essentially depends on the extrinsic geometry of the embedding $B \hookrightarrow \mathbb{R}^{d+k}$.

If we restrict $\mathring{M}$'s tangent bundle to M, one has the orthogonal decomposition

$$\mathsf{T}\mathring{M}|_M = \mathsf{T}M \oplus \mathsf{N}M \overset{(2.1)}{=} \mathsf{H}M \oplus \mathsf{V}M \oplus \mathsf{N}M \tag{5.1}$$

with respect to $\mathring{g}$. Due to the commutativity of the above diagram, it follows that $\mathsf{V}M \subset \mathsf{V}\mathring{M}|_M$. This suggests to introduce the notation $\mathsf{V}M^\perp$ for the orthogonal complement of $\mathsf{V}M$ in $\mathsf{V}\mathring{M}|_M$ with respect to $g_{\mathring{F}}$, i.e.

$$\mathsf{V}\mathring{M}|_M = \mathsf{V}M \oplus \mathsf{V}M^\perp. \tag{5.2}$$

For any $X \in \Gamma(\mathsf{T}B)$, let $X^{\mathsf{H}\mathring{M}} \in \Gamma(\mathsf{H}\mathring{M})$ and $X^{\mathsf{H}M} \in \Gamma(\mathsf{H}M)$ be the respective unique horizontal lifts. It then holds that

$$\pi_{\mathring{M}*}\big(X^{\mathsf{H}M} - X^{\mathsf{H}\mathring{M}}|_M\big) = \pi_{M*}X^{\mathsf{H}M} - \pi_{\mathring{M}*}X^{\mathsf{H}\mathring{M}}|_M = X - X = 0.$$

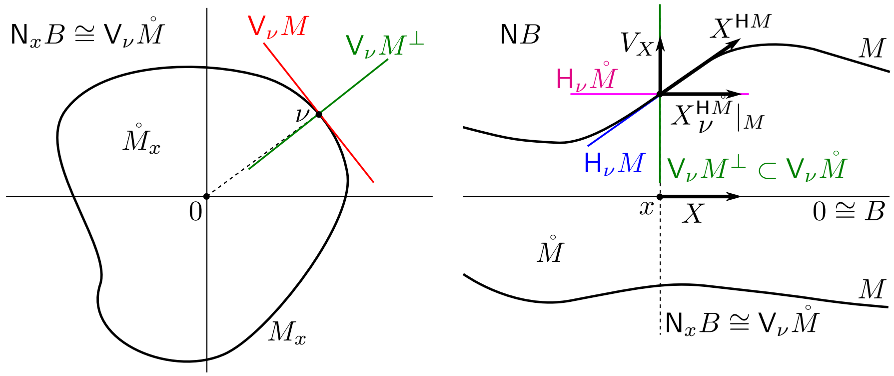

FIGURE 2. *Left* sketch of the fibre N_xB for any $x \in B$. Note that for any $\nu \in \mathring{M}_x \subset \mathsf{N}_xB$ we have the canonical identification of N_xB and $\mathsf{V}_\nu\mathring{M}$ via the isomorphism (4.4). *Right* relationship between the horizontal lifts $X^{\mathsf{H}M}$ and $X^{\mathsf{H}\mathring{M}}|_M$. They are connected by the vertical field V_X

Thus, the difference between $X^{\mathsf{H}M}$ and $X^{\mathsf{H}\mathring{M}}|_M$ is a vertical field:

$$X^{\mathsf{H}M} = X^{\mathsf{H}\mathring{M}}|_M + V_X \tag{5.3}$$

with $V_X \in \Gamma(\mathsf{V}\mathring{M}|_M)$. Moreover, $V_X \in \Gamma(\mathsf{V}M^\perp)$ since for arbitrary $W \in \Gamma(\mathsf{V}M) \subset \Gamma(\mathsf{V}\mathring{M}|_M)$

$$0 = g(X^{\mathsf{H}M}, W) = \underbrace{\mathring{g}\big(X^{\mathsf{H}\mathring{M}}|_M, W\big)}_{=0} + g_{\mathring{F}}\big(V_X, W\big)$$

implies $g_{\mathring{F}}(V_X, W) = 0$. The geometric situation is sketched in Fig. 2.

Obviously, the relation $\pi_{M*}X^{\mathsf{H}M} = X$ does not shed light on the vertical part V_X. The latter will be determined by the requirement $X^{\mathsf{H}M}$ to be a tangent vector field on M, or equivalently by the condition $\mathring{g}(X^{\mathsf{H}M}, n) = 0$, where $n \in \Gamma(\mathsf{N}M)$ denotes a unit normal field of M in $\mathring{M}$. To determine V_X from this condition, we first need to show that the vertical component of n is non-zero everywhere.

Lemma 5.1. *Let $n \in \Gamma(\mathsf{N}M)$ be a unit normal field of the hollow quantum waveguide M. Then, $v_n := \mathrm{P}^{\mathsf{V}\mathring{M}}\, n \in \Gamma(\mathsf{V}M^\perp)$ is a non-vanishing vector field.*

Proof. Decompose $n = v_n + h_n$ with $h_n := \mathrm{P}^{\mathsf{H}\mathring{M}}\, n \in \Gamma(\mathsf{H}\mathring{M}|_M)$. It then holds for any vector field $W \in \Gamma(\mathsf{V}M)$:

$$g_{\mathring{F}}(W, v_n) = \mathring{g}(W, v_n) = \mathring{g}(W, v_n + h_n) = \mathring{g}(W, n) = 0,$$

where we used (5.1) for the second and fourth equality. This clearly implies $v_n \in \Gamma(\mathsf{V}M^\perp)$ by (5.2). Now suppose there exists $\nu \in M$ with $v_n(\nu) = 0$. Consider the space

$$U_\nu := \mathsf{H}_\nu M \oplus \mathrm{span}\{(n(\nu)\} \subset \mathsf{T}_\nu\mathring{M}.$$

Since $n(\nu) \in \mathsf{N}_\nu M$ is orthogonal to $\mathsf{H}_\nu M \subset \mathsf{T}_\nu M$, one has $\dim(U_\nu) = d+1$. We will show that the kernel of $\pi_{\mathring{M}*}|_{U_\nu} : U_\nu \to \operatorname{im}(\pi_{\mathring{M}*}|_{U_\nu}) \subset \mathsf{T}_{\pi_{\mathring{M}}(\nu)}B$ is trivial. Hence,

$$d+1 = \dim(U_\nu) = \operatorname{rank}(\pi_{\mathring{M}*}|_{U_\nu}) \leq \dim\bigl(\mathsf{T}_{\pi_{\mathring{M}}(\nu)}B\bigr)$$

clearly contradicts the fact that $\dim(B) = d$ and finally the assumption that $n(\nu) = 0$. Therefore, let $w \in \ker(\pi_{\mathring{M}*}|_{U_\nu}) \in \mathsf{V}_\nu\mathring{M} \cap U_\nu$. On the one hand, since

$$n(\nu) = \underbrace{v_n(\nu)}_{=0} + h_n(\nu) \in \mathsf{H}_\nu\mathring{M} = \ker(\pi_{\mathring{M}*}|_\nu)^\perp,$$

w is an element of $\mathsf{H}_\nu M$. But on the other hand, $\pi_{\mathring{M}*}|_{\mathsf{H}_\nu M} : \mathsf{H}_\nu M \to \mathsf{T}_{\pi_{\mathring{M}}(\nu)}B$ possesses a trivial kernel. Together, this yields $w = 0$, i.e. $\ker(\pi_{\mathring{M}*}|_{U_\nu}) = \{0\}$. □

In view of Eq. (5.3), Lemma 5.1 suggests to define a function $\daleth(X) \in C^\infty(M)$ such that $V_X = \daleth(X)v_n$. Thus, the requirement $X^{\mathsf{H}M} \in \Gamma(\mathsf{T}M)$ yields

$$\begin{aligned} 0 = \mathring{g}(X^{\mathsf{H}M}, n) &= \mathring{g}\bigl(X^{\mathsf{H}\mathring{M}}|_M, n\bigr) + \mathring{g}(v_n, n)\daleth(X) \\ &= \mathring{g}^{\mathrm{hor}}\bigl(X^{\mathsf{H}\mathring{M}}|_M, h_n\bigr) + g_{\mathring{F}}(v_n, v_n)\daleth(X), \end{aligned}$$

consequently

$$\daleth(X) = -\frac{\mathring{g}^{\mathrm{hor}}(X^{\mathsf{H}\mathring{M}}|_M, h_n)}{g_{\mathring{F}}(v_n, v_n)}. \tag{5.4}$$

Note that $\daleth(X)$ is well defined since $g_{\mathring{F}}(v_n, v_n) > 0$ by Lemma 5.1. Moreover, the latter equation shows that $\daleth \in \mathcal{T}^0_1(B) \otimes C^\infty(M)$ is actually a tensor.

In summary, we just showed that the unscaled pullback metric on M may be written as:

$$g = g^{\mathrm{hor}} + g_F, \quad g_F := g_{\mathring{F}}|_{\mathsf{V}M}$$

with "horizontal block"

$$g^{\mathrm{hor}}(X^{\mathsf{H}M}, Y^{\mathsf{H}M}) := \mathring{g}^{\mathrm{hor}}\bigl(X^{\mathsf{H}\mathring{M}}|_M, Y^{\mathsf{H}\mathring{M}}|_M\bigr) + g_{\mathring{F}}(v_n, v_n)\daleth(X)\daleth(Y)$$

for $X, Y \in \Gamma(\mathsf{T}B)$. Going over to the scaled pullback metric g^ε, we first show that the horizontal lift remains unchanged.

Lemma 5.2. *Let $(M, g^\varepsilon) \to (B, g_B)$ be a hollow quantum waveguide for $\varepsilon > 0$. Then, the horizontal subbundle $\mathsf{H}M$ is independent of ε.*

Proof. It is sufficient to show that for any vector field $X \in \Gamma(\mathsf{T}B)$ its unique horizontal lift $X^{\mathsf{H}M}$ is given by the ε-independent expression

$$X^{\mathsf{H}M} = X^{\mathsf{H}\mathring{M}}|_M + \daleth(X)v_n$$

with $\daleth(X) \in C^\infty(M)$ and $v_n \in \Gamma(\mathsf{V}M^\perp)$ as before. We already know that $X^{\mathsf{H}M}$ is tangent to M and satisfies $\pi_{M*}X^{\mathsf{H}M} = X$. Thus, the requirement that $X^{\mathsf{H}M}$

is orthogonal to any $W \in \Gamma(\mathsf{V}M)$ with respect g^ε is the only possible way for any ε-dependence to come into play. Therefore, we calculate

$$\begin{aligned} & g^\varepsilon(X^{\mathsf{H}M}, W) \\ & = \mathring{g}^\varepsilon\big(X^{\mathsf{H}\mathring{M}}|_M + \daleth(X) v_n, W\big) \\ & = \underbrace{\varepsilon^{-2}\Big[\pi^*_{\mathring{M}} g_B\big(X^{\mathsf{H}\mathring{M}}|_M, W\big) + \varepsilon \mathring{h}^\varepsilon\big(X^{\mathsf{H}\mathring{M}}|_M, W\big)\Big]}_{=0,\ \text{since } W \in \Gamma(\mathsf{V}M) \subset \Gamma(\mathsf{V}\mathring{M}|_M)} + \daleth(X) \underbrace{g_{\mathring{F}}(v_n, W)}_{=0 \text{ by } (5.2)} \\ & = 0. \end{aligned}$$

□

In summary, if the scaled pullback metric of the massive waveguide $\mathring{M}$ has the form $\mathring{g}^\varepsilon = \varepsilon^{-2}(\pi^*_{\mathring{M}} g_B + \varepsilon \mathring{h}^\varepsilon) + g_{\mathring{F}}$, the scaled pullback metric g^ε of the associated hollow waveguide M reads

$$g^\varepsilon = \varepsilon^{-2}(\pi^*_M g_B + \varepsilon h^\varepsilon) + g_F \tag{5.5}$$

with

$$h^\varepsilon(X^{\mathsf{H}M}, Y^{\mathsf{H}M}) := \mathring{h}^\varepsilon\big(X^{\mathsf{H}\mathring{M}}|_M, Y^{\mathsf{H}\mathring{M}}|_M\big) + \varepsilon g_{\mathring{F}}(v_n, v_n) \daleth(X) \daleth(Y)$$

for $X, Y \in \Gamma(\mathsf{T}B)$. This shows that the scaled pullback metric g^ε is again of the form (2.2).

Example. Let us consider a simple example of a hollow quantum waveguide with $d = 1$, $k = 2$. Take $B = \{(x, 0, 0) \in \mathbb{R}^3 : \ x \in \mathbb{R}\} \subset \mathbb{R}^3$ as submanifold and parametrise the according massive quantum waveguide via

$$\mathring{M} := \Big\{(x, 0, 0) + \varrho\, r(x, \varphi) e_r : \ (x, \varphi, \varrho) \in \mathbb{R} \times [0, 2\pi) \times [0, 1]\Big\},$$

where $r : \mathbb{R} \times [0, 2\pi) \to [r_-, r_+]$ with $0 < r_- < r_+ < \infty$ is a smooth function obeying the periodicity condition $r(\cdot, \varphi + 2\pi) = r(\cdot, \varphi)$ and $e_r = (0, \cos\varphi, \sin\varphi) \in \mathsf{V}_{(x,\varphi,\varrho)}\mathring{M}$ stands for the “radial unit vector”. In view of Example 2 with $\kappa \equiv 0$, the unscaled pullback metric on $\mathring{M}$ is given by

$$\mathring{g} = \mathring{g}^{\text{hor}} + g_{\mathring{F}} = \mathrm{d}x^2 + (\varrho^2\, \mathrm{d}\varphi^2 + \mathrm{d}\varrho^2).$$

Furthermore, we immediately observe that $\mathsf{T}_x B = \operatorname{span}\{\partial_x\}$ with trivial horizontal lift $\partial_x^{\mathsf{H}\mathring{M}} = (1, 0, 0) =: e_x \in \mathsf{H}_{(x,\varphi,\varrho)}\mathring{M}$. The hollow quantum waveguide associated with M is obviously given by

$$M := \Big\{(x, 0, 0) + r(x, \varphi) e_r : \ (x, \varphi) \in \mathbb{R} \times [0, 2\pi)\Big\} = \mathring{M}|_{\varrho=1}.$$

Consequently, $\mathsf{T}_{(x,\varphi)}M$ is given by $\operatorname{span}\{\tau_x, \tau_\varphi\}$, where

$$\begin{aligned} \tau_x(x, \varphi) &= \tfrac{\partial M}{\partial x}(x, \varphi) = e_x + \tfrac{\partial r}{\partial x} e_r, \\ \tau_\varphi(x, \varphi) &= \tfrac{\partial M}{\partial \varphi}(x, \varphi) = \tfrac{\partial r}{\partial \varphi} e_r + r e_\varphi \end{aligned}$$

with $e_\varphi = (0, -\sin\varphi, \cos\varphi) \in \mathsf{V}_{(x,\varphi,\varrho)}\mathring{M}$. One easily agrees that τ_x and τ_φ are orthogonal to

$$\tilde{n} = -\tfrac{\partial r}{\partial \varphi} e_\varphi + r e_r - r \tfrac{\partial r}{\partial x} e_x$$

with respect to $\mathring{g}$. Hence

$$n(x,\varphi) := \frac{\tilde{n}}{\|\tilde{n}\|_{\mathring{g}}} = \underbrace{\frac{-\frac{\partial r}{\partial\varphi}e_\varphi + re_r}{\sqrt{(\frac{\partial r}{\partial\varphi})^2 + r^2\left[1+(\frac{\partial r}{\partial x})^2\right]}}}_{=:v_n \in \mathsf{V}_{(x,\varphi)}M^\perp} + \underbrace{\frac{-r\frac{\partial r}{\partial x}e_x}{\sqrt{(\frac{\partial r}{\partial\varphi})^2 + r^2\left[1+(\frac{\partial r}{\partial x})^2\right]}}}_{=:h_n \in \mathsf{H}_{(x,\varphi)}\mathring{M}}$$

is a unit normal vector of M at (x,φ) for $\varepsilon = 1$. Noting that

$$g_{\mathring{F}}(v_n, v_n) = \frac{(\frac{\partial r}{\partial\varphi})^2 + r^2}{(\frac{\partial r}{\partial\varphi})^2 + r^2\left[1+(\frac{\partial r}{\partial x})^2\right]},$$

Equation (5.4) gives

$$\begin{aligned}
\daleth(\partial_x) &= -\frac{\mathring{g}^{\mathrm{hor}}(\partial_x^{\mathsf{H}\mathring{M}}|_M, h_n)}{g_{\mathring{F}}(v_n,v_n)} \\
&= -\frac{-r\frac{\partial r}{\partial\varphi}}{\sqrt{(\frac{\partial r}{\partial\varphi})^2 + r^2\left[1+(\frac{\partial r}{\partial x})^2\right]}}\left(\frac{(\frac{\partial r}{\partial\varphi})^2 + r^2}{(\frac{\partial r}{\partial\varphi})^2 + r^2\left[1+(\frac{\partial r}{\partial x})^2\right]}\right)^{-1} \\
&= \frac{r\frac{\partial r}{\partial\varphi}\sqrt{(\frac{\partial r}{\partial\varphi})^2 + r^2\left[1+(\frac{\partial r}{\partial x})^2\right]}}{(\frac{\partial r}{\partial\varphi})^2 + r^2}.
\end{aligned}$$

This yields the following expression for the "horizontal block" of the scaled pullback metric g^ε:

$$\begin{aligned}
g^{\varepsilon,\mathrm{hor}}(\partial_x^{\mathsf{H}M}, \partial_x^{\mathsf{H}M}) &= \varepsilon^{-2}\,\mathrm{d}x^2\big(\partial_x^{\mathsf{H}\mathring{M}}|_M, \partial_x^{\mathsf{H}\mathring{M}}|_M\big) + g_{\mathring{F}}(v_n,v_n)\daleth(\partial_x)\daleth(\partial_x) \\
&= \varepsilon^{-2} + \frac{r^2(\frac{\partial r}{\partial x})^2}{(\frac{\partial r}{\partial\varphi})^2 + r^2} \\
&= \varepsilon^{-2}\big(1 + \varepsilon h^\varepsilon(\partial_x^{\mathsf{H}M}, \partial_x^{\mathsf{H}M})\big)
\end{aligned}$$

with

$$h^\varepsilon(\partial_x^{\mathsf{H}M}, \partial_x^{\mathsf{H}M}) = \varepsilon\frac{r^2(\frac{\partial r}{\partial x})^2}{(\frac{\partial r}{\partial\varphi})^2 + r^2}.$$

5.2. The Adiabatic Hamiltonian

We now calculate the adiabatic operator for hollow waveguides. Since in this case the fibre is a manifold without boundary, the ground state of H_F is explicitly known:

$$\phi_0 = \sqrt{\frac{\rho_\varepsilon}{\|\rho_\varepsilon\|_1}} = \pi_M^*\operatorname{Vol}(F_x)^{-1/2} + \mathcal{O}(\varepsilon),$$

where $\|\rho_\varepsilon\|_1(x)$ is the L^1-norm of ρ_ε on the fibre F_x. Because of this, we can express many of the terms appearing in H_a, given in Eq. (3.3), through ρ_ε.

Let us begin with the sum of the modified bending potential $\tilde{V}_{\mathrm{bend}}$ appearing in H_1 and the adiabatic potential V_a. First, we obtain an expression for the one-form $\bar{\eta}$ by observing that for any vector field X on B

$$0 = X \int_{F_x} |\phi_0|^2 \; \mathrm{d}g_F = \int_{F_x} X^{\mathsf{H}M} |\phi_0|^2 \; \mathrm{d}g_F - \underbrace{\int_{F_x} |\phi_0|^2 \, g_B(X, \pi_{M*}\eta_F) \, \mathrm{d}g_F}_{=\bar{\eta}(X)}.$$

So we see that

$$\bar{\eta} = \int_{F_x} \mathrm{P}^{\mathsf{H}M}\big(\mathrm{d}|\phi_0|^2\big) \; \mathrm{d}g_F. \tag{5.6}$$

Now to start with the first term of the adiabatic potential can be calculated as in (4.16)

$$\begin{aligned}
\mathrm{tr}_{g_B}(\nabla^B \bar{\eta}) &= \mathrm{div}_{g_B}\, g_B(\bar{\eta}, \cdot) \\
&\overset{(4.9)}{=} \int_{F_x} \mathrm{div}_{g_s}\big(\mathrm{P}^{\mathsf{H}M}\, \mathrm{grad}_{g_s} |\phi_0|^2\big) \; \mathrm{d}g_F \\
&\overset{(2.4)}{=} \int_{F_x} \Delta_{\mathsf{H}} |\phi_0|^2 \; \mathrm{d}g_F.
\end{aligned}$$

For the modified bending potential one has, using the shorthand $|F_x| = \mathrm{Vol}(F_x)$,

$$\begin{aligned}
\varepsilon^2 \tilde{V}^{\mathrm{a}}_{\mathrm{bend}} &:= P_0\big(V_{\mathrm{bend}} - \tfrac{1}{2}\Delta_{\mathsf{V}}(\log \rho_\varepsilon) - \tfrac{1}{4} g_F(\mathrm{d}\log\rho_\varepsilon, \mathrm{d}\log\rho_\varepsilon)\big) P_0 \\
&= \frac{\varepsilon^2}{2} \int_{F_x} |\phi_0|^2 \, \Delta_{\mathsf{H}}(\log \rho_\varepsilon) \; \mathrm{d}g_F + \mathcal{O}(\varepsilon^4) \\
&= \frac{\varepsilon^2}{2} \int_{F_x} |F_x|^{-1} \, (\Delta_{\mathsf{H}} \rho_\varepsilon) \; \mathrm{d}g_F + \mathcal{O}(\varepsilon^4).
\end{aligned}$$

Note that this expression is of order ε^3 since $\rho_\varepsilon = 1 + \mathcal{O}(\varepsilon)$. Hence, bending does not contribute to the leading order of H_{a}. Now inserting the explicit form of ϕ_0 an elementary calculation yields

$$\begin{aligned}
V_{\mathrm{a}} + \tilde{V}^{\mathrm{a}}_{\mathrm{bend}} = \int_{F_x} & -\tfrac{1}{2}\rho_\varepsilon \Delta_{\mathsf{H}} \|\rho_\varepsilon\|_1^{-1} - \tfrac{1}{2} g_B\big(\mathrm{grad}\, |F_x|^{-1}, \pi_{M*}\, \mathrm{grad}\, \rho_\varepsilon\big) \\
& + \tfrac{1}{4}\rho_\varepsilon \, \|\rho_\varepsilon\|_1 \, g_B\big(\pi_{M*}\, \mathrm{grad}\, \|\rho_\varepsilon\|_1^{-1}, \pi_{M*}\, \mathrm{grad}\, \|\rho_\varepsilon\|_1^{-1}\big) \; \mathrm{d}g_F \\
& + \mathcal{O}(\varepsilon^2).
\end{aligned} \tag{5.7}$$

With $\rho_\varepsilon = 1 + \mathcal{O}(\varepsilon)$ and $\|\rho_\varepsilon\|_1 = |F_x| + \mathcal{O}(\varepsilon)$ one easily checks that up to order ε this expression equals

$$\tfrac{1}{4} g_B\big(\mathrm{d}\log |F_x|, \mathrm{d}\log |F_x|\big) + \tfrac{1}{2}\Delta_{g_B} \log |F_x|.$$

As far as the remaining terms of H_1 are concerned, note that the scaled pull-back metric g^ε of the hollow waveguide has the same expansion on horizontal one-forms up to errors of order ε^4 as in the case of the massive waveguide (4.13), i.e.

$$g^\varepsilon(\pi_M^* \mathrm{d}x^i, \pi_M^* \mathrm{d}x^j) = \varepsilon^2\big(g_B^{ij} + 2\varepsilon\, \mathrm{II}(\nu)^{ij} + \mathcal{O}(\varepsilon^2)\big).$$

Hence, we can calculate these terms starting from expression (4.15). Since the latter all carry a prefactor ε^3, we may replace any ϕ_0 by $|F_x|^{-1/2}$, obtaining for $\psi \in L^2(B)$

$$\int_{F_x} \operatorname{div}_{g_s}\left(|\phi_0|^2 \operatorname{II}(\nu)(\mathrm{d}\psi,\cdot)\right)\,\mathrm{d}g_F = \int_{F_x} \operatorname{div}_{g_s}\left(|F_x|^{-1} \operatorname{II}(\nu)(\mathrm{d}\psi,\cdot)\right)\,\mathrm{d}g_F + \mathcal{O}(\varepsilon) \tag{5.8}$$

and

$$\begin{aligned}\int_{F_x} \phi_0 \operatorname{div}_{g_s}\left(\operatorname{II}(\nu)(\pi_{M*}\operatorname{grad}_{g_s}\phi_0,\cdot)\right)\,\mathrm{d}g_F \\ = \int_{F_x} |F_x|^{-1/2} \operatorname{div}_{g_s}\left(\operatorname{II}(\nu)\left(\mathrm{d}\,|F_x|^{-1/2},\cdot\right)\right)\,\mathrm{d}g_F + \mathcal{O}(\varepsilon).\end{aligned} \tag{5.9}$$

As in Eq. (4.16), we have

$$\int_{F_x} \operatorname{div}_{g_s}\left(|F_x|^{-1} \operatorname{II}(\nu)(\mathrm{d}\psi,\cdot)\right)\,\mathrm{d}g_F = \operatorname{div}_{g_B} \int_{F_x} |F_x|^{-1} \operatorname{II}(\nu)(\mathrm{d}\psi,\cdot)\,\mathrm{d}g_F.$$

Again, this term vanishes if the barycentre of the fibres $F_x = \partial\mathring{F}_x \subset \mathsf{N}_x B$ is zero, that is

$$\int_{F_x} \nu\,\mathrm{d}g_F = 0.$$

Since $\lambda_0 \equiv 0$, the adiabatic operator is of the form

$$\begin{aligned}H_{\mathrm{a}} &= -\varepsilon^2\Delta_{g_B} + \varepsilon^2 V_{\mathrm{a}} + \varepsilon P_0 H_1 P_0 \\ &= -\varepsilon^2\Delta_{g_B} + \varepsilon^2\Big(\tfrac{1}{4} g_B\left(\mathrm{d}\log|F_x|\,,\mathrm{d}\log|F_x|\right) + \tfrac{1}{2}\Delta_{g_B}\log|F_x|\Big) + \mathcal{O}(\varepsilon^3),\end{aligned} \tag{5.10}$$

with an error in $\mathcal{L}(W^2(B), L^2(B))$. Thus, the adiabatic operator at leading order is just the Laplacian on the base B plus an effective potential depending solely on the relative change of the volume of the fibres. Going one order further in the approximation, we have

$$\varepsilon^2 V_{\mathrm{a}} + \varepsilon P_0 H_1 P_0 = \varepsilon^2(5.7) + 2\varepsilon^3(5.9) + 2\varepsilon^3(5.8) + \mathcal{O}(\varepsilon^4)$$

in the same norm. Hence, H_{a} also contains the second order differential operator (5.8) if the barycentre of F_x is different from zero. Let us also remark that the leading order of the adiabatic potential can also be calculated by applying a unitary transformation $L^2(F, \mathrm{d}g_F) \to L^2(F, |F_x|^{-1}\,\mathrm{d}g_F)$ that rescales fibre volume to one, in the spirit of $\mathcal{M}_{\rho_\varepsilon}$ [cf. Eq. (2.5)]. In this way a similar potential was derived by Kleine [9], in a slightly different context, for a special case with one-dimensional base and without bending.

References

[1] Bouchitté, G., Mascarenhas, M.L., Trabucho, L.: On the curvature and torsion effects in one dimensional waveguides. ESAIM: Control Optim. Calc. of Var. **13**, 793–808 (2007)

[2] Bishop, R.L.: There is more than one way to frame a curve. Am. Math. Mon. **82**, 246–251 (1975)

[3] Carron, G., Exner, P., Krejčiřík, D.: Topologically nontrivial quantum layers. J. Math. Phys. **45**, 774–784 (2004)

[4] da Costa, R.: Constraints in quantum mechanics. Phys. Rev. A **25**, 2893–2900 (1982)

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

[6] Ekholm, T., Kovařík, H., Krejčiřík, D.: A Hardy inequality in twisted waveguides. Arch. Ration. Mech. Anal. **188**, 245–264 (2008)

[7] Froese, R., Herbst, I.: Realizing holonomic constraints in classical and quantum mechanics. Commun. Math. Phys. **220**, 489–535 (2001)

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

[9] Kleine, R.: Discreteness conditions for the Laplacian on complete, non-compact Riemannian manifolds. Mathematische Zeitschrift **198**, 127–141 (1988)

[10] Krejčiřík, D.: Twisting versus bending in quantum waveguides. In: Analysis on Graphs and its Applications: Proceedings of the Symposium on Pure Mathematics, pp. 617–636. American Mathematical Society, Providence (2008)

[11] Krejčiřík, D., Lu, Z.: Location of the essential spectrum in curved quantum layers. arXiv:1211.2541 (2012)

[12] Krejčiřík, D., Raymond, N.: Magnetic effects in curved quantum waveguides. arXiv:1303.6844 (2013)

[13] Krejčiřík, D., Raymond, N., Tušek, M.: The magnetic Laplacian in shrinking tubular neighbourhoods of hypersurfaces. arXiv:1303.4753 (2013)

[14] Krejčiřík, D., Šediváková, H.: The effective Hamiltonian in curved quantum waveguides under mild regularity assumptions. Rev. Math. Phys. **24**, 1250018 (2012)

[15] Lampart, J.: The adiabatic limit of Schrödinger operators on fibre bundles. PhD thesis, Eberhard Karls Universität Tübingen (2014)

[16] Lampart, J., Teufel, S.: The adiabatic limit of Schrödinger operators on fibre bundles. arXiv:1402.0382 (2014)

[17] Lampart, J., Teufel, S., Wachsmuth, J.: Effective Hamiltonians for thin Dirichlet tubes with varying cross-section. In: Mathematical Results in Quantum Physics: Proceedings of the QMath11 Conference, pp. 183–189. World Scientific Publishing Co., Singapore (2011)

[18] Lin, C., Lu, Z.: On the discrete spectrum of generalized quantum tubes. Commun. Partial Differ. Equ. **31**, 1529–1546 (2006)

[19] Maraner, P.: A complete perturbative expansion for quantum mechanics with constraints. J. Phys. A Math. Gen. **28**, 2939–2951 (1995)

[20] Mitchell, K.A.: Gauge fields and extrapotentials in constrained quantum systems. Phys. Rev. A **63**, 042112 (2001)

[21] de Oliveira, G.: Quantum dynamics of a particle constrained to lie on a surface. arXiv:1310.6651 (2013)

[22] de Oliveira, C.R., Verri, A.A.: On the spectrum and weakly effective operator for Dirichlet Laplacian in thin deformed tubes. J. Math. Anal. Appl. **381**, 454–468 (2011)

[23] Panati, G., Spohn, H., Teufel, S.: Space-adiabatic pertubation theory. Adv. Theor. Math. Phys. **7**, 145–204 (2003)

[24] Schick, T.: Analysis on ∂-Manifolds of Bounded Geometry, Hodge-de Rham Isomorphism and L^2-Index Theorem. PhD thesis, Johannes Gutenberg Universität Mainz (1996)

[25] Stockhofe, J., Schmelcher, P.: Curved quantum waveguides: Nonadiabatic couplings and gauge theoretical structure. Phys. Rev. A **89**, 033630 (2014)

[26] Teufel, S.: Adiabatic pertubation theory in quantum dynamics. Lecture Notes in Mathematics, vol. 1821. Springer, Berlin (2003)

[27] Tolar, J.: On a quantum mechanical d'Alembert principle. Lecture Notes in Physics, vol. 313. Springer, Berlin (1988)

[28] Wachsmuth, J., Teufel, S.: Effective Hamiltonians for constrained quantum systems. Mem. Am. Math. Soc. **230** (2013)

[29] Wittich, O.: A homogenization result for Laplacians on tubular neighbourhoods of closed Riemannian submanifolds. Habilitation Treatise, Eberhard Karls Universität Tübingen (2007)

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