

Effective Dynamics for Constrained Quantum Systems

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Abstract

We consider the time dependent Schrödinger equation on a Riemannian manifold \mathcal{A} with a potential that localizes a certain class of states close to a fixed submanifold \mathcal{C} , the constraint manifold. When we scale the potential in the directions normal to \mathcal{C} by a parameter $\varepsilon \ll 1$, the solutions concentrate in an ε -neighborhood of the submanifold. We derive an effective Schrödinger equation on the submanifold \mathcal{C} and show that its solutions, suitably lifted to \mathcal{A} , approximate the solutions of the original equation on \mathcal{A} up to errors of order $\varepsilon^3|t|$ at time t .

Our result holds in the situation where tangential and normal energies are of the same order, and where exchange between normal and tangential energies occurs. In earlier results tangential energies were assumed to be small compared to normal energies, and rather restrictive assumptions were needed, to ensure that the separation of energies is maintained during the time evolution. Most importantly, we can now allow for constraining potentials that change their shape along the submanifold, which is the typical situation in applications like molecular dynamics and quantum waveguides.

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1 Introduction

Although the mathematical structure of the linear Schrödinger equation

$$i\partial_t\psi = -\Delta\psi + V\psi =: H\psi, \quad \psi|_{t=0} \in L^2(\mathcal{A}, d\tau) \quad (1)$$

is quite simple, in many cases the high dimension of the underlying configuration space \mathcal{A} makes even a numerical solution impossible. Therefore it is important to identify situations where the dimension can be reduced by approximating the solutions of the original equation (1) on the high dimensional configuration space \mathcal{A} by solutions of an *effective equation*

$$i\partial_t\phi = H_{\text{eff}}\phi, \quad \phi|_{t=0} \in L^2(\mathcal{C}, d\mu) \quad (2)$$

on a lower dimensional configuration space \mathcal{C} .

The physically most straightforward situation where such a dimensional reduction is possible are constrained mechanical systems. In these systems strong forces effectively constrain the system to remain in the vicinity of a submanifold \mathcal{C} of the configuration space \mathcal{A} .

For classical Hamiltonian systems there is a straightforward mathematical reduction procedure. One just projects the Hamiltonian vector field from the tangent bundle of $T^*\mathcal{A}$ to the tangent bundle of $T^*\mathcal{C}$ and then studies its dynamics on $T^*\mathcal{C}$. For quantum systems Dirac [9] proposed to quantize the restricted classical Hamiltonian system on the submanifold following an “intrinsic” quantization procedure. However, for curved submanifolds \mathcal{C} there is no unique quantization procedure. One natural guess would be an effective Hamiltonian H_{eff} in (2) of the form

$$H_{\text{eff}} = -\Delta_{\mathcal{C}} + V|_{\mathcal{C}}, \quad (3)$$

where $\Delta_{\mathcal{C}}$ is the Laplace-Beltrami operator on \mathcal{C} with respect to the induced metric and $V|_{\mathcal{C}}$ is the restriction of the potential $V : \mathcal{A} \rightarrow \mathbb{R}$ to \mathcal{C} .

However, to justify or invalidate the above procedures from first principles, one needs to model the constraining forces within the dynamics (1) on the full space \mathcal{A} . This is done by adding a localizing part to the potential V . Then one analyzes the behavior of solutions of (1) in the asymptotic limit where the constraining forces become very strong and tries to extract a suitable limiting equation on \mathcal{C} . This limit of strong confining forces has been studied in classical mechanics and in quantum mechanics many times in the literature. The classical case was first investigated by Rubin-Ungar [30], who found that in the limiting dynamics an extra potential appears that accounts for the energy contained in the normal oscillations. Today there is a wide literature on the subject. We mention the monograph by Bornemann [2] for a result based on weak convergence and a survey and the book of Hairer, Lubich and Wanner [15], Section XIV.3, for an approach based on classical adiabatic invariants.

For the quantum mechanical case Marcus [21] and later on Jensen and Koppe [17] pointed out that the limiting dynamics depends, in addition, also on the embedding of the submanifold \mathcal{C} into the ambient space \mathcal{A} . In the sequel Da Costa [6] deduced a geometrical condition (often called the no-twist condition) ensuring that the effective dynamics does not depend on the localizing potential. This condition is equivalent to the flatness of the normal bundle of \mathcal{C} . It fails to hold for a generic submanifold of dimension and codimension both strictly greater than one, which is a typical situation when applying these ideas to molecular dynamics.

Thus the hope to obtain a generic “intrinsic” effective dynamics as in (3), i.e. a Hamiltonian that depends only on the intrinsic geometry of \mathcal{C} and

the restriction of the potential V to \mathcal{C} , is unfounded. In both, classical and quantum mechanics, the limiting dynamics on the constraint manifold depends, in general, on the detailed nature of the constraining forces, on the embedding of \mathcal{C} into \mathcal{A} and on the initial data. In our paper we present and prove a general result concerning the precise form of the limiting dynamics (2) on \mathcal{C} starting from (1) on the ambient space \mathcal{A} with a strongly confining potential V . However, as we explain next, our result generalizes existing results in the mathematical and physical literature not only on a technical level, but improves the range of applicability in a deeper sense.

Da Costa's statement (like the more refined results by Froese-Herbst [13], Maraner [19] and Mitchell [23], which we discuss in Subsection 1.2) requires that the constraining potential is the same at each point on the submanifold. The reason behind this assumption is that the energy stored in the normal modes diverges in the limit of strong confinement. As in the classical result by Rubin and Ungar, variations in the constraining potential lead to exchange of energy between normal and tangential modes, and thus also the energy in the tangential direction grows in the limit of strong confinement. However, the problem can be treated without adiabatic methods only for solutions with bounded kinetic energies in the tangential directions. Therefore the transfer of energy between normal and tangential modes was excluded in [6, 19, 13, 23] by the assumption that the confining potential has the same shape in the normal direction at any point of the submanifold. In many important applications this assumption is violated, for example for the reaction paths of molecular reactions. The reaction valleys vary in shape depending on the configuration of the nuclei. In the same applications also the typical normal and tangential energies are of the same order.

Therefore the most important new aspect of our result is that we allow for confining potentials that vary in shape and for solutions with normal and tangential energies of the same order. As a consequence, our limiting dynamics on the constraint manifold has a richer structure than earlier results and resembles, at leading order, the results from classical mechanics. In the limit of small tangential energies we recover the limiting dynamics by Mitchell [23].

The key observation for our analysis is that the problem is an adiabatic limit and has, at least locally, a structure similar to the Born-Oppenheimer approximation in molecular dynamics. In particular, we transfer ideas from adiabatic perturbation theory, which were developed by Nenciu-Martinez-Sordani and Panati-Spohn-Teufel in [22, 25, 27, 33, 35], to a non-flat geometry. We note that the adiabatic nature of the problem was observed many times before in the physics literature, e.g. in the context of adiabatic quantum wave guides [5], but we are not aware of any work considering constraint

manifolds with general geometries in quantum mechanics from this point of view. In particular, we believe that our effective equations have not been derived or guessed before and are new not only as a mathematical but also as a physics result. In the mathematics literature we are aware of two predecessor works: in [35] the problem was solved for constraint manifolds \mathcal{C} which are d -dimensional subspaces of \mathbb{R}^{d+k} , while Dell'Antonio and Tenuta [8] considered the leading order behavior of semiclassical Gaussian wave packets for general geometries.

Another result about submanifolds of arbitrary dimension is due to Wittich [36], who considers the heat equation on thin tubes of manifolds. Finally, there are related results in the wide literature on thin tubes of quantum graphs. A good starting point for it is [14] by Grieser, where mathematical techniques used in this context are reviewed. Both works and the papers cited there, properly translated, deal with the case of small tangential energies.

We now give a nontechnical and short sketch of the structure of our result. The detailed statements from Section 2 require some preparation.

We implement the limit of strong confinement by mapping the problem to the normal bundle $N\mathcal{C}$ of \mathcal{C} and then scaling one part of the potential in the normal direction by ε^{-1} . With decreasing ε the normal derivatives of the potential and thus the constraining forces increase. In order to obtain a nontrivial scaling behavior of the equation, the Laplacian is multiplied with a prefactor ε^2 . The reasoning behind this scaling, which is the same as in [13, 23], is explained in Section 1.2. With q denoting coordinates on \mathcal{C} and ν denoting normal coordinates our starting equation on $N\mathcal{C}$ has, still somewhat formally, the form

$$i\partial_t\psi^\varepsilon = -\varepsilon^2\Delta_{N\mathcal{C}}\psi^\varepsilon + V(q, \varepsilon^{-1}\nu)\psi^\varepsilon + W(q, \nu)\psi^\varepsilon =: H^\varepsilon\psi^\varepsilon \quad (4)$$

for $\psi^\varepsilon|_{t=0} \in L^2(N\mathcal{C})$. Here $\Delta_{N\mathcal{C}}$ is the Laplace-Beltrami operator on $N\mathcal{C}$, where the metric on $N\mathcal{C}$ is obtained by pulling back the metric on a tubular neighborhood of \mathcal{C} in \mathcal{A} to a tubular neighborhood of the zero section in $N\mathcal{C}$ and then suitably extending it to all of $N\mathcal{C}$. We study the asymptotic behavior of (4) as ε goes to zero uniformly for initial data with energies of order one. This means that initial data are allowed to oscillate on a scale of order ε not only in the normal direction, but also in the tangential direction, i.e. that tangential kinetic energies are of the same order as the normal energies. More precisely, we assume that $\|\varepsilon\nabla^h\psi_0^\varepsilon\|^2 = \langle\psi_0^\varepsilon | -\varepsilon^2\Delta_h\psi_0^\varepsilon\rangle$ is of order one, in contrast to the earlier works [13, 23], where it was assumed to be of order ε^2 . Here ∇^h is a suitable horizontal derivative to be introduced in Definition 1.

Our final result is basically an effective equation of the form (2). It is presented in two steps. In Theorem 1 we show that on certain subspaces of

$L^2(N\mathcal{C})$ the unitary group $\exp(-iH^\varepsilon t)$ generating solutions of (4) is unitarily equivalent to an “effective” unitary group $\exp(-iH_{\text{eff}}^\varepsilon t)$ associated to (2) up to errors of order $\varepsilon^3|t|$ uniformly for bounded initial energies. In Theorem 2 we compute the asymptotic expansion of $H_{\text{eff}}^\varepsilon$ up to terms of order ε^2 , i.e. we compute $H_{\text{eff},0}$, $H_{\text{eff},1}$ and $H_{\text{eff},2}$ in $H_{\text{eff}} = H_{\text{eff},0} + \varepsilon H_{\text{eff},1} + \varepsilon^2 H_{\text{eff},2} + \mathcal{O}(\varepsilon^3)$. The first step in our proof is the construction of closed infinite dimensional subspaces of $L^2(N\mathcal{C})$ which are invariant under the dynamics (4) up to small errors and which can be mapped unitarily to $L^2(\mathcal{C})$, where the effective dynamics takes place. To construct these “almost invariant subspaces”, we define at each point q of \mathcal{C} a normal Hamiltonian operator $H_f(q)$ acting on the fibre $N_q\mathcal{C}$. If it has a simple eigenvalue band $E(q)$ depending smoothly on q and being isolated from the rest of the spectrum for all q , then the corresponding eigenspaces define a smooth line bundle over \mathcal{C} . Its L^2 -sections define a closed subspace of $L^2(N\mathcal{C})$, which after a modification of order ε becomes the almost invariant subspace associated to the eigenvalue band $E(q)$. In the end, to each isolated eigenvalue band $E(q)$ there is an associated line bundle over \mathcal{C} , an associated almost invariant subspace and an associated effective Hamiltonian $H_{\text{eff}}^\varepsilon$.

We now come to the form of the effective Hamiltonian associated to an isolated eigenvalue band $E(q)$. For $H_{\text{eff},0}$ we obtain, as expected, the Laplace-Beltrami operator of the submanifold as kinetic energy term and as an additional effective potential the eigenvalue band $E(q)$,

$$H_{\text{eff},0} = -\varepsilon^2 \Delta_{\mathcal{C}} + E.$$

Note that $V|_{\mathcal{C}}$ is contained in E . This is the quantum version of the classical mechanics result of Rubin and Ungar [30]. However, the time scale for which the solutions of (4) propagate along finite distances are times t of order ε^{-1} . On this longer time scale the first order correction $\varepsilon H_{\text{eff},1}$ to the effective Hamiltonian has effects of order one and must be included in the effective dynamics. We don’t give the details of $H_{\text{eff},1}$ here and just mention that at next to leading order the kinetic energy term, i.e. the Laplace-Beltrami operator, must be modified in two ways. First, the metric on \mathcal{C} needs to be changed by terms of order ε depending on exterior curvature, whenever the center of mass of the normal eigenfunctions does not lie exactly on the submanifold \mathcal{C} . Furthermore, the connection on the trivial line bundle over \mathcal{C} (where the wave function ϕ takes its values) must be changed from the trivial to a generalized Berry connection. This is because the normal eigenfunction may vary in shape along the submanifold and thus the line bundle associated to the eigenvalue band $E(q)$ inherits a nontrivial induced connection, the Berry connection. This was already discussed by Mitchell in the case that the potential (and thus the eigenfunctions) only twists.

The second order corrections in $H_{\text{eff},2}$ are quite numerous. In addition to terms similar to those at first order, we find generalizations of the Born-Huang potential and the off-band coupling both known from the Born-Oppenheimer setting, and an extra potential depending on inner and exterior curvature, whose occurrence lead to Marcus' reply to Dirac's proposal. Finally when the ambient space is not flat, there is another extra potential already obtained by Mitchell.

Note that in the earlier works it was assumed that $-\varepsilon^2\Delta_{\mathcal{C}}$ is of order ε^2 and thus of the same size as the terms in $H_{\text{eff},2}$. This is why the extra potential depending on curvature appeared at leading order in these works, while it appears only in $H_{\text{eff},2}$ for us. And this is also the reason that assumptions were necessary, assuring that all other terms appearing in our $H_{\text{eff},0}$ and $H_{\text{eff},1}$ are of higher order or trivial, including that $E(q) \equiv E$ is constant.

We end this section with some more technical comments concerning our result and the difficulties encountered in its proof.

In this work we present the result only for simple eigenvalues $E(q)$. With one caveat, it extends to degenerate eigenvalues in a straightforward way. Our construction requires the complex line bundle associated with $E(q)$ to be trivializable. For line bundles, triviality follows from the vanishing of the first Chern class. And for real Hamiltonians like H^ε in (4) it turns out that the complex line bundle associated to $E(q)$ always has vanishing first Chern class. However, for degenerate eigenvalue bands no such argument is available (except for a compact \mathcal{C} with $\dim\mathcal{C} \leq 3$, see Panati [26]) and we would have to add triviality of the associated bundle to our assumptions. Moreover, for degenerate bands the statements and proofs would become even more lengthy, which is why we restricted ourselves to the case of simple eigenvalue bands $E(q)$. Generalizations to not necessary real Hamiltonians containing also magnetic fields are in preparation.

Next let us emphasize that we do not assume the potential to become large away from the submanifold. That means we achieve the confinement solely through large potential gradients, not through high potential barriers. This leads to several additional technical difficulties, not encountered in other rigorous results on the topic that mostly consider harmonic constraints. One aspect of this is the fact that the normal Hamiltonian $H_f(q)$ has also continuous spectrum. While its eigenfunctions defining the adiabatic subspaces decay exponentially, the superadiabatic subspaces, which are relevant for our analysis, are slightly tilted spectral subspaces with small components in the continuous spectral subspace.

Let us finally mention two technical lemmas, which may both be of independent interest. After extending the pull back metric from a tubular neigh-

borhood of \mathcal{C} in \mathcal{A} to the whole normal bundle, with this metric NC has curvature increasing linearly with the distance from \mathcal{C} . As a consequence we have to prove weighted elliptic estimates for a manifold of unbounded curvature (Lemmas 9 & 10). Moreover, since we aim at uniform results we need to introduce energy cutoffs. A result of possibly wider applicability is that the smoothing by energy cutoffs preserves polynomial decay (Lemma 13).

1.1 The model

Let (\mathcal{A}, G) be a Riemannian manifold of dimension $d+k$ ($d, k \in \mathbb{N}$) with associated volume measure $d\tau$. Let furthermore $\mathcal{C} \subset \mathcal{A}$ be a smooth submanifold without boundary and of dimension $d/\text{codimension } k$, which is equipped with the induced metric $g = G|_{\mathcal{C}}$ and volume measure $d\mu$. We will call \mathcal{A} the *ambient manifold* and \mathcal{C} the *constraint manifold*.

On \mathcal{C} there is a natural decomposition $T\mathcal{A}|_{\mathcal{C}} = T\mathcal{C} \times NC$ of \mathcal{A} 's tangent bundle into the tangent and the normal bundle of \mathcal{C} . We assume that there exists a tubular neighbourhood $\mathcal{B} \subset \mathcal{A}$ of \mathcal{C} with globally fixed diameter, that is there is $\delta > 0$ such that normal geodesics γ (i.e. $\gamma(0) \in \mathcal{C}, \dot{\gamma}(0) \in NC$) of length δ do not intersect. We will call a tubular neighbourhood of radius r an *r-tube*. Furthermore we assume that

$$\mathcal{B} \text{ and } \mathcal{C} \text{ are of bounded geometry} \quad (5)$$

(see the appendix for the definition) and that the embedding

$$\mathcal{C} \hookrightarrow \mathcal{A} \text{ has globally bounded derivatives of any order,} \quad (6)$$

where boundedness is measured by the metric G ! In particular, these assumptions are satisfied for $\mathcal{A} = \mathbb{R}^{d+k}$ and a smoothly embedded \mathcal{C} that is (a covering of) a compact manifold or asymptotically flatly embedded, which are the cases arising mostly in the applications we are interested in (molecular dynamics and quantum waveguides).

Let $\Delta_{\mathcal{A}}$ be the Laplace-Beltrami operator on \mathcal{A} . We want to study the Schrödinger equation

$$i\partial_t\psi = -\Delta_{\mathcal{A}}\psi + V_{\mathcal{A}}^{\varepsilon}\psi, \quad \psi|_{t=0} \in L^2(\mathcal{A}, d\tau), \quad (7)$$

under the assumption that the potential $V_{\mathcal{A}}^{\varepsilon}$ localizes at least a certain class of states in an ε -tube of \mathcal{C} with $\varepsilon \ll \delta$. The localization will be realized by simply imposing that the potential is squeezed like ε^{-1} in the directions normal to the submanifold. We emphasize that we will not assume $V_{\mathcal{A}}^{\varepsilon}$ to become large, which makes the proof of localization more difficult.

In order to actually implement the scaling in the normal direction, we will now construct a related problem on the normal bundle of \mathcal{C} by mapping $N\mathcal{C}$ diffeomorphically to the tubular neighbourhood \mathcal{B} of \mathcal{C} in a specific way and then choosing a suitable metric \bar{g} on $N\mathcal{C}$ (considered as a manifold). On the normal bundle the scaling of the potential in the normal directions is straightforward. The theorem we prove for the normal bundle will later be translated back to the original setting. On a first reading it may be convenient to skip the technical construction of \bar{g} and of the horizontal and vertical derivatives ∇^h and ∇^v and to immediately jump to the end of Definition 1.

The mapping to the normal bundle is done in the following way. There is a natural diffeomorphism from the δ -tube \mathcal{B} to the δ -neighbourhood \mathcal{B}_δ of the zero section of the normal bundle $N\mathcal{C}$. This diffeomorphism corresponds to choosing coordinates on \mathcal{B} that are geodesic in the directions normal to \mathcal{C} . These coordinates are often called (generalized) Fermi coordinates. They will be examined in detail in Section 4.2. In the following we will always identify \mathcal{C} with the zero section of the normal bundle. Next we choose any diffeomorphism $\tilde{\Phi} \in C^\infty(\mathbb{R}, (-\delta, \delta))$ which is the identity on $(-\delta/2, \delta/2)$ and satisfies

$$\forall j \in \mathbb{N} \quad \exists C_j < \infty \quad \forall r \in \mathbb{R} : \quad |\tilde{\Phi}^{(j)}(r)| \leq C_j (1 + r^2)^{-(j+1)/2}, \quad (8)$$

(see Figure 1). Then a diffeomorphism $\Phi \in C^\infty(N\mathcal{C}, \mathcal{B}_\delta)$ is obtained by first applying $\tilde{\Phi}$ to the radial coordinate on each fibre $N_q\mathcal{C}$ (which are all isomorphic to \mathbb{R}^k) and then using Fermi coordinate charts.

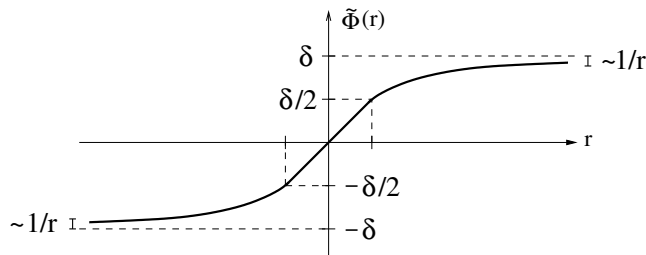


Figure 1: $\tilde{\Phi}$ converges to $\pm\delta$ like $1/r$.

The important step now is to choose a suitable metric and corresponding measure on $N\mathcal{C}$. On the one hand we want it to be the pullback of G on $\mathcal{B}_{\delta/4}$. On the other hand, we require that the distance to \mathcal{C} asymptotically behaves like the radius in each fibre and that the associated volume measure on $N\mathcal{C} \setminus \mathcal{B}_{\delta/2}$ is $d\mu \otimes d\nu$, where $d\nu$ is the Lebesgue measure on the fibers of $N\mathcal{C}$ and $d\mu \otimes d\nu$ is the product measure (the Lebesgue measure and the product measure are defined after locally choosing an orthonormal trivializing frame

of NC ; they do not depend on the choice of the trivialization because the Lebesgue measure is isotropic). The latter two requirements will help to obtain the decay that is needed to translate the result back to \mathcal{A} .

A metric satisfying the two latter properties globally is the so-called Sasaki metric which is defined in the following way (see e.g. [1]): The Levi Civita connection on \mathcal{A} induces a connection ∇ on $T\mathcal{C}$, which is the Levi-Civita connection on (\mathcal{C}, g) , and a connection ∇^\perp on NC which is called the *normal connection* (see the appendix). Let $\pi : NC \rightarrow \mathcal{C}$ be the bundle projection and $K : TNC \rightarrow NC$ be the connection map induced by the normal connection ∇^\perp . The Sasaki metric is then given by

$$g_{(q,\nu)}^S(v, w) := g_q(D\pi v, D\pi w) + G_{(q,0)}(Kv, Kw). \quad (9)$$

It was studied by Wittich in [36] in a similar context. Due to the sum structure, the completeness of (NC, g^S) follows from the completeness of the fibers and the completeness of \mathcal{C} . The latter holds, because \mathcal{C} is of bounded geometry. In spite of this (NC, g^S) is in general not of bounded geometry, however, $(\mathcal{B}_\delta, g^S)$ is. Both can be seen directly from the formulas for the curvature in [1]. Now we simply fade the pullback metric into the Sasaki metric by defining

$$\bar{g}_{(q,\nu)}(v, w) := \Theta(|\nu|) G_{\Phi(q,\nu)}(D\Phi v, D\Phi w) + (1 - \Theta(|\nu|)) g_{(q,\nu)}^S(v, w) \quad (10)$$

with $|\nu| := \sqrt{G_{\Phi(q,0)}(D\Phi\nu, D\Phi\nu)}$ and a cutoff function $\Theta \in C^\infty([0, \infty), [0, 1])$ satisfying $\Theta \equiv 1$ on $[0, \delta/4]$ and $\Theta \equiv 0$ on $[\delta/2, \infty)$. Then we have

$$|\nu| = \sqrt{\bar{g}_{(q,0)}(\nu, \nu)}. \quad (11)$$

The Levi-Civita connection on (NC, \bar{g}) will be denoted by $\bar{\nabla}$ and the volume measure associated to \bar{g} by $d\bar{\mu}$. We note that \mathcal{C} is still isometrically imbedded and that (NC, \bar{g}) is complete due to the bounded geometry of (\mathcal{B}_δ, G) and the completeness of (NC, g^S) . Furthermore \bar{g} induces the same connections ∇ and ∇^\perp on $T\mathcal{C}$ and NC as G .

The volume measure associated to g^S is indeed $d\mu \otimes d\nu$ and its density with respect to the measure associated to G equals 1 on \mathcal{C} (see Section 6.1 of [36]). Together with the bounded geometry of (\mathcal{B}_δ, G) and of $(\mathcal{B}_\delta, g^S)$ we obtain that

$$\frac{d\bar{\mu}}{d\mu \otimes d\nu} \Big|_{(NC \setminus \mathcal{B}_{\delta/2}) \cup \mathcal{C}} \equiv 1, \quad \frac{d\bar{\mu}}{d\mu \otimes d\nu} \in C_b^\infty(NC), \quad \frac{d\bar{\mu}}{d\mu \otimes d\nu} \geq c > 0, \quad (12)$$

where $C_b^\infty(NC)$ is the space of smooth functions on NC with all its derivatives globally bounded with respect to \bar{g} .

Since we will think of the functions on NC as mappings from \mathcal{C} to the functions on the fibers, the following derivative operators will play a crucial role.

Definition 1 Denote by $\Gamma(\mathcal{E})$ the set of all smooth sections of a bundle \mathcal{E} and by $\Gamma_b(\mathcal{E})$ the ones with globally bounded derivatives up to any order.

i) Fix $q \in \mathcal{C}$. The fiber $(N_q\mathcal{C}, \bar{g}_{(q,0)})$ is isometric to the euclidean \mathbb{R}^k . Therefore there is a canonical identification ι of normal vectors at $q \in \mathcal{C}$ with tangent vectors at $(q, \nu) \in N_q\mathcal{C}$. The vertical derivative $\nabla^\nu\varphi$ at (q, ν) is the pullback via ι of the exterior derivative of φ 's restriction to $N_q\mathcal{C}$, i.e.

$$\nabla_\zeta^\nu\varphi(q, \nu) = (d\varphi_{(q,\nu)})(\iota(\zeta))$$

for $\zeta \in \Gamma(N\mathcal{C})$. The Laplacian associated to $-\int_{N_q\mathcal{C}} \bar{g}_{(q,0)}(\nabla^\nu\varphi, \nabla^\nu\varphi) d\nu$ is denoted by Δ_ν and the set of bounded functions with bounded derivatives of arbitrary order by $C_b^\infty(N_q\mathcal{C})$.

ii) Let $\mathcal{E} := \{(q, \varphi) \mid q \in \mathcal{C}, \varphi \in C_b^\infty(N_q\mathcal{C})\}$ be the bundle over \mathcal{C} which is obtained by replacing the fibers $N_q\mathcal{C}$ of the normal bundle with $C_b^\infty(N_q\mathcal{C})$ and canonically lifting the bundle structure of $N\mathcal{C}$. Let $\varphi : \mathcal{C} \rightarrow \mathcal{E}$ be a section, i.e. $\varphi_q \in C_b^\infty(N_q\mathcal{C})$. The horizontal connection $\nabla^h : \Gamma(T\mathcal{C}) \times \Gamma(\mathcal{E}) \rightarrow \Gamma(\mathcal{E})$ on \mathcal{E} is defined by

$$\nabla_\tau^h\varphi_q(\nu) := \left. \frac{d}{ds} \right|_{s=0} \varphi(w(s), v(s)), \quad (13)$$

where $\tau \in \Gamma(T\mathcal{C})$ and $(w, v) \in C^1([-1, 1], N\mathcal{C})$ with

$$w(0) = q, \quad \dot{w}(0) = \tau(q), \quad \& \quad v(0) = \nu, \quad \nabla_w^\perp v = 0.$$

Furthermore Δ_h is the Bochner Laplacian associated to ∇^h :

$$\int_{N\mathcal{C}} \psi^* \Delta_h \psi \, d\mu \otimes d\nu = - \int_{N\mathcal{C}} g(\nabla^h \psi^*, \nabla^h \psi) \, d\mu \otimes d\nu,$$

where we have used the same letter g for the canonical shift of g to the cotangent bundle. Higher order horizontal derivatives are inductively defined by

$$\nabla_{\tau_1, \dots, \tau_m}^h \varphi := \nabla_{\tau_1}^h \nabla_{\tau_2, \dots, \tau_m}^h \varphi - \sum_{j=2}^m \nabla_{\tau_2, \dots, \nabla_{\tau_1} \tau_j, \dots, \tau_m}^h \varphi$$

for arbitrary $\tau_1, \dots, \tau_m \in \Gamma(T\mathcal{C})$. The set of bounded sections φ of \mathcal{E} such that $\nabla_{\tau_1, \dots, \tau_m}^h \varphi$ is also a bounded section for all $\tau_1, \dots, \tau_m \in \Gamma_b(T\mathcal{C})$ is denoted by $C_b^m(\mathcal{C}, C_b^\infty(N_q\mathcal{C}))$.

In the sequel we consider the complex Hilbert space $\bar{\mathcal{H}} := L^2((N\mathcal{C}, \bar{g}), d\bar{\mu})$. We emphasize that elements of $\bar{\mathcal{H}}$ take values in the trivial complex line bundle over $N\mathcal{C}$. This will be the case for all functions throughout this paper

and we will omit this in the definition of Hilbert spaces. However, there will come up non-trivial connections on such line bundles! In addition, we notice that the Riemannian metrics on $N\mathcal{C}$ and \mathcal{C} have canonical continuations on the associated trivial complex line bundles.

The scalar product of a Hilbert space \mathcal{H} will be denoted by $\langle \cdot | \cdot \rangle_{\mathcal{H}}$ and the induced norm by $\| \cdot \|_{\mathcal{H}}$. The upper index $*$ will be used for both the adjoint of an operator and the conjugation of a function.

Instead of (7) we now consider a Schrödinger equation on the normal bundle thought of as a Riemannian manifold $(N\mathcal{C}, \bar{g})$. Here we can immediately implement the idea of squeezing the potential in the normal directions: Let

$$V^\varepsilon(q, \nu) = V_c(q, \varepsilon^{-1}\nu) + W(q, \nu)$$

for fixed real-valued potentials $V_c, W \in C_b^\infty(\mathcal{C}, C_b^\infty(N_q\mathcal{C}))$. Here we have split up any $Q \in N\mathcal{C}$ as (q, ν) where $q \in \mathcal{C}$ is the base point and ν is a vector in the fiber $N_q\mathcal{C}$ at q . We allow for an “external potential” W which does not contribute to the confinement and is not scaled. Then $\varepsilon \ll 1$ corresponds to the regime of strong confining forces. The setting is sketched in Figure 2.

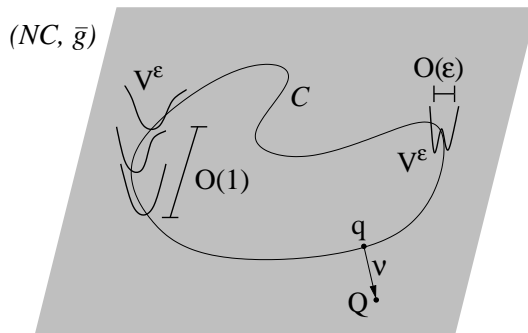


Figure 2: The width of V_ε is ε but it varies on a scale of order one along \mathcal{C} .

We will investigate the Schrödinger equation

$$i\partial_t\psi = H^\varepsilon\psi := -\varepsilon^2\Delta_{N\mathcal{C}}\psi + V^\varepsilon\psi, \quad \psi|_{t=0} = \psi_0^\varepsilon \in \bar{\mathcal{H}}, \quad (14)$$

where $\Delta_{N\mathcal{C}}$ is the Laplace operator on $(N\mathcal{C}, \bar{g})$, i.e. the operator associated to $-\int_{N\mathcal{C}} \bar{g}(d\psi, d\psi)d\bar{\mu}$. To ensure proper scaling behavior, we need to multiply the Laplacian in (14) by ε^2 . The physical meaning of this is explained at the end of the next subsection. Here we only emphasize that an analogous scaling was used implicitly or explicitly in all other previous works on the problem of constraints in quantum mechanics. The crucial difference in our work is, as explained before, that we allow ε -dependent initial data ψ_0^ε with tangential kinetic energy $\langle \psi_0^\varepsilon | -\varepsilon^2\Delta_{N\mathcal{C}}\psi_0^\varepsilon \rangle$ of order one instead of order ε^2 .

The operator H^ε will be called the Hamiltonian. We note that H^ε is real, i.e. it maps real-valued functions to real-valued functions. Furthermore it is bounded from below because we assumed V_c and W to be bounded. In [32] H^ε is shown to be selfadjoint on the Sobolev space $H^2(\mathcal{M})$ (defined by patching together local Sobolev spaces) for any complete Riemannian manifold \mathcal{M} , thus in particular for (NC, \bar{g}) .

We only need one additional assumption on the potential, that ensures localization in normal direction. Before we state it, we clarify the structure of adiabatic separation:

After a unitary transformation H^ε can at leading order be split up into an operator which acts on the fibers only and a horizontal operator. That unitary transformation M_ρ is given by multiplication with the square root of the relative density $\rho := \frac{d\bar{\mu}}{d\mu \otimes d\nu}$ of our starting measure and the product measure on NC that was introduced above. We recall from (12) that this density is bounded and strictly positive. After the transformation it is helpful to rescale the normal directions.

Definition 2 Set $\mathcal{H} := L^2(NC, d\mu \otimes d\nu)$ and $\rho := \frac{d\bar{\mu}}{d\mu \otimes d\nu}$.

- i) The unitary transform M_ρ is defined by $M_\rho : \mathcal{H} \rightarrow \overline{\mathcal{H}}, \psi \mapsto \rho^{\frac{1}{2}}\psi$.
- ii) The dilation operator D_ε is defined by $(D_\varepsilon\psi)(q, \nu) := \varepsilon^{-k/2}\psi(q, \nu/\varepsilon)$.
- iii) The dilated Hamiltonian H_ε and potential V_ε are defined by

$$H_\varepsilon := D_\varepsilon^* M_\rho^* H^\varepsilon M_\rho D_\varepsilon, \quad V_\varepsilon := D_\varepsilon^* M_\rho^* V^\varepsilon M_\rho D_\varepsilon = V_c + D_\varepsilon^* W D_\varepsilon.$$

The index ε will consistently be placed down to denote dilated objects, while it will be placed up to denote objects in the original scale.

The leading order of H_ε will turn out to be the sum of $-\Delta_v + V_c(q, \cdot) + W(q, 0)$ and $-\varepsilon^2\Delta_h$ (for details on M_ρ and the expansion of H_ε see Lemmas 1 & 4 below). When $-\varepsilon^2\Delta_h$ acts on functions that are constant on each fibre, it is simply the Laplace-Beltrami operator on \mathcal{C} carrying an ε^2 . Hereby the analogy with the Born-Oppenheimer setting is revealed where the kinetic energy of the nuclei carries the small parameter given by the ratio of the electron mass and the nucleon mass (see for example [27]).

We need that the family of q -dependent operators $-\Delta_v + V_c(q, \cdot) + W(q, 0)$ has a family of exponentially decaying bound states in order to construct a class of states that are localized close to the constraint manifold. The following definition makes this precise. We note that the conditions are simpler to verify than one might have thought in the manifold setting, since the space and the operators involved are euclidean!

Definition 3 Let $\mathcal{H}_f(q) := L^2(N_q\mathcal{C}, d\nu)$ and $V_0(q, \nu) := V_c(q, \nu) + W(q, 0)$. The selfadjoint operator $(H_f(q), H^2(N_q\mathcal{C}, d\nu))$ with

$$H_f(q) := -\Delta_\nu + V_0(q, \cdot) \quad (15)$$

is called the fiber Hamiltonian. Its spectrum is denoted by $\sigma(H_f(q))$.

i) A function $E_0 : \mathcal{C} \rightarrow \mathbb{C}$ is called an energy band, if $E_0(q) \in \sigma(H_f(q))$ for all $q \in \mathcal{C}$. E_0 is called simple, if $E_0(q)$ is a simple eigenvalue for all $q \in \mathcal{C}$.

ii) An energy band $E_0 : \mathcal{C} \rightarrow \mathbb{C}$ is called separated, if there are a constant $c_{\text{gap}} > 0$ and two bounded continuous functions $f_\pm : \mathcal{C} \rightarrow \mathbb{R}$ defining an interval $I(q) := [f_-(q), f_+(q)]$ such that

$$E_0(q) \subset I(q), \quad \inf_{q \in \mathcal{C}} \text{dist}(\sigma(H_f(q)) \setminus E_0(q), I(q)) = c_{\text{gap}}. \quad (16)$$

iii) A separated energy band E_0 is called a constraint energy band, if there is $\Lambda_0 > 0$ such that the family of spectral projections $P_0 : \mathcal{C} \rightarrow \mathcal{L}(\mathcal{H}_f(q))$ corresponding to E_0 satisfies

$$\sup_{q \in \mathcal{C}} \|e^{\Lambda_0 \langle \nu \rangle} P_0(q) e^{\Lambda_0 \langle \nu \rangle}\|_{\mathcal{L}(\mathcal{H}_f(q))} < \infty,$$

where $\langle \nu \rangle := \sqrt{1 + |\nu|^2} = \sqrt{1 + \bar{g}_{(q,0)}(\nu, \nu)}$.

We emphasize that condition ii) is known to imply condition iii) in lots of cases, for example for eigenvalues below the continuous spectrum (see [16] for a review of known results). Besides, condition ii) is a uniform but local condition (see Figure 3).

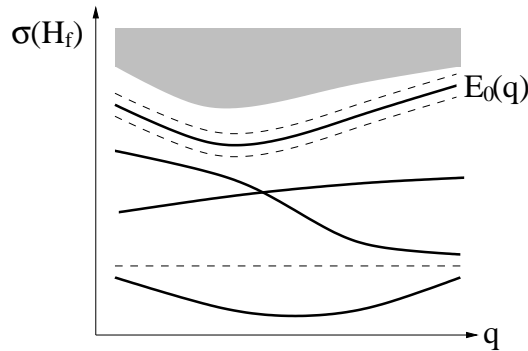


Figure 3: $E_0(q)$ has to be separated by a local gap that is uniform in q .

A family of spectral projections $P_0 : \mathcal{C} \rightarrow \mathcal{L}(\mathcal{H}_f(q))$ of rank one corresponds to a line bundle over \mathcal{C} . If this bundle has a global section $\varphi_0 : \mathcal{C} \rightarrow \mathcal{H}_f(q)$

of normalized eigenfunctions, $(P_0\psi)(q) = \langle \varphi_0 | \psi \rangle_{\mathcal{H}_\varepsilon(q)} \varphi_0(q)$ for all $q \in \mathcal{C}$. Furthermore φ_0 can be used to define a unitary mapping U_0 between the corresponding subspace $P_0\mathcal{H}$ and $L^2(\mathcal{C}, d\mu)$ by

$$(U_0\psi)(q) := \langle \varphi_0 | \psi \rangle_{\mathcal{H}_\varepsilon(q)}.$$

So any $\psi \in P_0\mathcal{H}$ has the product structure $\psi = (U_0\psi)\varphi_0$. Since V_0 and therefore φ_0 depends on q , such a product will in general not be invariant under the time evolution. However, it will turn out to be at least approximately invariant. For short times this follows from the fact that the commutator $[H_\varepsilon, P_0] = [-\varepsilon^2\Delta_h, P_0] + \mathcal{O}(\varepsilon)$ is of order ε . For long times this is a consequence of adiabatic decoupling.

On the macroscopic scale the corresponding eigenfunction $D_\varepsilon\varphi_0$ is more and more localized close to the submanifold: most of its mass is contained in the ε -tube around \mathcal{C} and it decays like $e^{\Lambda_0|\zeta|/\varepsilon}$. This is visualized in Figure 4.

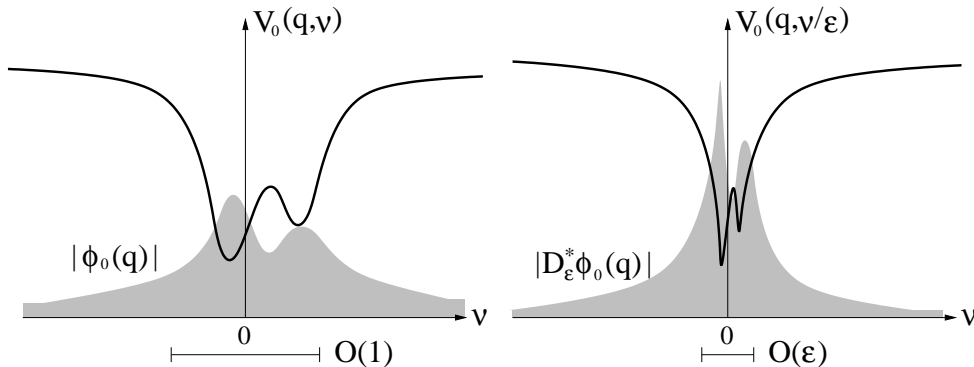


Figure 4: On the macroscopic level φ_0 is localized on a scale of order ε .

Our goal is to obtain an effective equation of motion on the submanifold for states that are localized close to the submanifold in that sense. More precisely, for each subspace $P_0\mathcal{H}$ corresponding to a constraint energy band E_0 we will derive an effective equation using the map U_0 . However, in order to control errors with higher accuracy we will have to add corrections of order ε to $P_0\mathcal{H}$ and U_0 .

1.2 Comparison with existing results

Since similar settings have been considered several times in the past, we want to point out the similarities and the differences with respect to our result. We mostly focus on the papers by Mitchell [23] and Froese-Herbst [13], since [23] is the most general one on a theoretical physics level and [13] is the

only mathematical paper concerned with deriving effective dynamics on the constraint manifold. Both works deal with a Hamiltonian that is of the form

$$\tilde{H}^\varepsilon = -\Delta_{NC} + \varepsilon^{-2}V_c^\varepsilon + W. \quad (17)$$

The confining potential V_c^ε is chosen to be the same everywhere on \mathcal{C} up to rotations, i.e. in any local bundle chart (q, ν) there exists a smooth family of rotations $R(q) \in \text{SO}(k)$ such that

$$V_c^\varepsilon(q, \nu) = V_c(q, \varepsilon^{-1}\nu) = V_c(q_0, \varepsilon^{-1}R(q)\nu)$$

for some fixed point q_0 on \mathcal{C} . As a consequence, the eigenvalues of the resulting fiber Hamiltonian $H_f(q) = -\Delta_\nu + V_c(q, \cdot)$ are constant, $E(q) \equiv E$. As our Theorems 1 and 2, the final result in [23] and somewhat disguised also in [13] is about effective Hamiltonians acting on $L^2(\mathcal{C})$ which approximate the full dynamics on corresponding subspaces of $L^2(N\mathcal{C})$. In the following we explain how the results in [13, 23] about (17) are related to our results on the seemingly different problem (14). It turns out that they indeed follow from our general results under the special assumptions on the confining potential and in a low energy limit.

To see this and to better understand the meaning of the scaling, note that when we multiply \tilde{H}^ε by ε^2 , the resulting Hamiltonian

$$\varepsilon^2 \tilde{H}^\varepsilon = -\varepsilon^2 \Delta_{NC} + V_c^\varepsilon + \varepsilon^2 W,$$

is the same as H^ε in (14), however, with very restrictive assumptions on the confining part V_c and with a non-confining part of order ε^2 . As one also has to multiply the left hand side of the Schrödinger equation (14) by ε^2 , this should be interpreted in the following way. Results valid for times of order one for the group generated by \tilde{H}^ε would be valid for times of order ε^{-2} for the group generated by $\varepsilon^2 \tilde{H}^\varepsilon$. On this time scale our result still yields an approximation with small errors (of order ε). Thus the results in [13, 23] are valid on the same physical time scale as ours.

We look at (14) for initial data with horizontal kinetic energies $\langle \psi_0^\varepsilon | -\varepsilon^2 \Delta_h \psi_0^\varepsilon \rangle$ of order one. This corresponds to horizontal kinetic energies $\langle \psi_0^\varepsilon | -\Delta_h \psi_0^\varepsilon \rangle$ of order ε^{-2} in (17), i.e. to the situation where potential and kinetic energies are of the same order. However, in [13, 19, 23] it is assumed that horizontal kinetic energies are of order one, i.e. smaller by a factor ε^2 than the potential energies. And to ensure that the horizontal kinetic energies remain bounded during the time evolution, the huge effective potential $\varepsilon^{-2}E(q)$ given by the normal eigenvalue must be constant. This is achieved in [13, 19, 23] by assuming that, up to rotations, the confining potential is the same everywhere on \mathcal{C} .

Technically, the assumption that (in our units) $\langle \psi_0^\varepsilon | -\varepsilon^2 \Delta_{\mathbf{h}} \psi_0^\varepsilon \rangle$ is of order ε^2 simplifies the analysis significantly. This is because the first step in proving effective dynamics for states in a subspace $P_0 \mathcal{H}$ for times of order ε^{-2} is to prove that it is approximately invariant under the time evolution for such times. Now the above assumption implies that the commutator $[H^\varepsilon, P_0]$ is of order ε^2 , and, as a direct consequence, that the subspace $P_0 \mathcal{H}$ is approximately invariant up to times of order ε^{-1} ,

$$\| [e^{-iH^\varepsilon t}, P_0] \| = \mathcal{O}(\varepsilon^2 |t|).$$

To get approximate invariance for times of order ε^{-2} one still needs an additional adiabatic argument, which is missing in [23]. Still, the result in [23] is correct for the same reason that the textbook derivation of the Born-Oppenheimer approximation is incomplete but yields the correct result including the first order Berry connection term. In [13] it is observed that one either has to assume spherical symmetry of the confining potential, which implies that $[H_\varepsilon, P_0]$ is of order ε^3 , or that one has to do an additional averaging argument in order to determine an effective Hamiltonian valid for times of order ε^{-2} . For our case of large kinetic energies the simple argument just gives

$$\| [e^{-iH^\varepsilon t}, P_0] \| = \mathcal{O}(\varepsilon |t|).$$

Therefore we need to replace the adiabatic subspaces $P_0 \mathcal{H}$ by so called super-adiabatic subspaces $P^\varepsilon \mathcal{H}$ in order to pass to the relevant time scale.

We end the introduction with a short discussion on the physical meaning of the scaling. While it is natural to model strong confining forces by dilating the confining potential in the normal direction, the question remains, why in (17) there appears the factor ε^{-2} in front of the confining potential, or, in our units, why there appears the factor ε^2 in front of the Laplacian in (14). The short answer is that without this factor no solutions of the corresponding Schrödinger equation would exist that remain ε -close to \mathcal{C} . Any solution initially localized in a ε -tube around \mathcal{C} would immediately spread out because its normal kinetic energy would be of order ε^{-2} , allowing it to overcome any confining potential of order one. Thus by the prefactor ε^{-2} in (17) the confining potential is scaled to the level of normal kinetic energies for ε -localized solutions, while in (14) we instead bring down the normal kinetic energy of ε -localized solutions to the level of the finite potential energies.

The longer answer forces us to look at the physical situation for which we want to derive asymptotically correct effective equations. The prime examples where our results are relevant are molecular dynamics, which was the motivation for [19, 20, 23], and nanotubes and -films (see e.g. [5]). In both cases one is not interested in the situation of infinite confining forces and

perfect constraints. One rather has a regime where the confining potential is given and fixed by the physics, but where the variation of all other potentials and of the geometry is small on the scale defined by the confining potential. This is exactly the regime described by the asymptotics $\varepsilon \ll 1$ in (14).

2 Main results

2.1 Effective dynamics on the constraint manifold

Since the potential V_c is varying along the submanifold, the normal and the tangential dynamics do not decouple completely at leading order and, as explained above, the product structure of states in $P_0\mathcal{H}$ is not invariant under the time evolution. In order to get a higher order approximation valid also for times of order ε^{-2} , we need to work on so-called superadiabatic subspaces $P_\varepsilon\mathcal{H}$. These are close to the adiabatic subspaces $P_0\mathcal{H}$ in the sense that the corresponding projections P_ε have an expansion in ε starting with the projection P_0 .

Furthermore when there is a global orthonormal frame of the eigenspace bundle defined by $P_0(q)$, the dynamics inside the superadiabatic subspaces can be mapped unitarily to dynamics on a space over the submanifold only.

We restrict ourselves here to a simple energy band, i.e. with one-dimensional eigenspaces. This circumvents an eventual topological non-triviality:

Remark 1 *If $E_0 : \mathcal{C} \rightarrow \mathbb{R}$ is a simple constraint energy band (as defined in Definition 3), then the corresponding eigenspace bundle has a smooth global section $\varphi_0 : \mathcal{C} \rightarrow \mathcal{H}_f(q)$ of normalized eigenfunctions. Furthermore the operator $U_0 : \mathcal{H} \rightarrow L^2(\mathcal{C}, d\mu)$ defined by $(U_0\psi)(q) := \langle \varphi_0 | \psi \rangle(q)$ satisfies*

$$U_0^*U_0 = P_0 \quad \& \quad U_0U_0^* = 1,$$

where U_0^* is given by $U_0^*\psi = \varphi_0\psi$ for all $\psi \in L^2(\mathcal{C}, d\mu)$.

To see this we notice that the eigenfunctions of $H_f(q)$ can be chosen real-valued because $H_f(q)$ is a real operator for all $q \in \mathcal{C}$. So we deal with a bundle that is the complexification of a real bundle. The first integer Chern class of a complexified bundle always vanishes (see e.g. [3]). For a line bundle this already means that the bundle is trivializable due to a classical result (see e.g. 2.1.3. in [4]). That is why we can choose a global normalized section φ_0 . We mention that Panati [26] showed that for a compact \mathcal{C} with $d \leq 3$ the triviality also follows from the vanishing of the first integer Chern class.

Of course we could also simply assume the existence of a trivializing frame. However, we do not want to overburden the result about the effective Hamiltonian (Theorem 2). Generalizations to the case of non-trivializable bundles are the subject of present work.

Theorem 1 *Fix $E < \infty$. Let $V_c, W \in C_b^\infty(\mathcal{C}, C_b^\infty(N_q\mathcal{C}))$ and E_0 be a simple constraint energy band.*

Then there are $C < \infty$ and $\varepsilon_0 > 0$ such that for all $\varepsilon < \varepsilon_0$ there are

- *a closed subspace $\mathcal{P}^\varepsilon\overline{\mathcal{H}} \subset \overline{\mathcal{H}}$ with orthogonal projection \mathcal{P}^ε ,*
- *a Riemannian metric $g_{\text{eff}}^\varepsilon$ on \mathcal{C} with associated measure $d\mu_{\text{eff}}^\varepsilon$,*
- *a unitary mapping $\mathcal{U}^\varepsilon : \mathcal{P}^\varepsilon\overline{\mathcal{H}} \rightarrow L^2(\mathcal{C}, d\mu_{\text{eff}}^\varepsilon)$,*
- *and a self-adjoint operator $H_{\text{eff}}^\varepsilon$ on $L^2(\mathcal{C}, d\mu_{\text{eff}}^\varepsilon)$*

which satisfy

$$\| (e^{-iH^\varepsilon t} - \mathcal{U}^{\varepsilon*} e^{-iH_{\text{eff}}^\varepsilon t} \mathcal{U}^\varepsilon) \mathcal{P}^\varepsilon \chi(H^\varepsilon) \|_{\mathcal{L}(\overline{\mathcal{H}})} < C \varepsilon^3 |t| \quad (18)$$

for all $t \in \mathbb{R}$ and each characteristic function χ with $\text{supp } \chi \subset (-\infty, E]$. Here $\chi(H^\varepsilon)$ is defined via the spectral theorem. Furthermore

$$\| (e^{-iH^\varepsilon t} - \mathcal{U}_0^{\varepsilon*} e^{-iH_{\text{eff}}^\varepsilon t} \mathcal{U}_0^\varepsilon) \mathcal{P}_0^\varepsilon \chi(H^\varepsilon) \|_{\mathcal{L}(\overline{\mathcal{H}})} < C \varepsilon (\varepsilon^2 |t| + 1), \quad (19)$$

where $\mathcal{U}_0^\varepsilon := U_0 D_\varepsilon^$ and $\mathcal{P}_0^\varepsilon := D_\varepsilon P_0 D_\varepsilon^*$.*

The proof of this result can be found in Section 3.1. The result (18) means that, after cutting off large energies, the superadiabatic subspace $\mathcal{P}^\varepsilon\overline{\mathcal{H}}$ is invariant up to errors of order $\varepsilon^3|t|$ and that on this subspace the unitary group $e^{-iH^\varepsilon t}$ on $L^2(N\mathcal{C})$ is unitarily equivalent to the effective unitary group $e^{-iH_{\text{eff}}^\varepsilon t}$ on $L^2(\mathcal{C})$ with the same error. In particular, there is adiabatic decoupling of the horizontal and vertical dynamics. We note that the energy cutoff $\chi(H^\varepsilon)$ is necessary in order to obtain a uniform error estimate, since the adiabatic decoupling breaks down for large energies because of the quadratic dispersion relation. It should be also pointed out here that, while $\mathcal{P}^\varepsilon \chi(H^\varepsilon)$ is not a projection, $\| \mathcal{P}^\varepsilon \chi(H^\varepsilon) \psi \| \geq (1 - c\varepsilon) \| \psi \|$ for a $c < \infty$ independent of ε on the relevant subspace $\mathcal{U}^* \tilde{\chi}(H_{\text{eff}}^\varepsilon) L^2(\mathcal{C}, d\mu_{\text{eff}}^\varepsilon)$ for $\tilde{\chi}$ with slightly smaller support than χ (follows from Lemma 6 below).

The result (19) follows from (18) by replacing \mathcal{P}^ε and \mathcal{U}^ε by their leading order expressions $\mathcal{P}_0^\varepsilon$ and $\mathcal{U}_0^\varepsilon$, which adds a time independent error of order ε . While somewhat weaker, the result (19) is much better suited for applications, since $\mathcal{P}_0^\varepsilon$ and $\mathcal{U}_0^\varepsilon$ are explicitly given in terms of the eigenfunction φ_0

and depend on ε only through the scaling by D_ε . Moreover, as we will see in Theorem 2, an asymptotic expansion of $H_{\text{eff}}^\varepsilon$ including all relevant terms can be computed explicitly as well.

Before we come to the effective Hamiltonian, we note that the above result about effective dynamics for NC will imply an analogous result on \mathcal{A} .

Definition 4 Set $A\psi := \left(\frac{d\bar{\mu}}{\Phi^*d\tau}\right)^{1/2} (\psi \circ \Phi)$ with $\Phi : NC \rightarrow \mathcal{B}_\delta$ as constructed in Section 1.1 and $\Phi^*d\tau$ the pullback of $d\tau$ via Φ . This defines an operator $A \in \mathcal{L}(L^2(\mathcal{A}, d\tau), \overline{\mathcal{H}})$ with $AA^* = 1$.

The stated properties of A are easily verified by using the substitution rule.

Corollary 1 Fix $\delta > 0$ and $E < \infty$. Let $H_{\mathcal{A}}^\varepsilon := -\varepsilon^2 \Delta_{\mathcal{A}} + V_{\mathcal{A}}^\varepsilon$ be self-adjoint on $L^2(\mathcal{A}, d\tau)$. Assume that $V^\varepsilon := AV_{\mathcal{A}}^\varepsilon A^*$ satisfies the assumptions from Theorem 1. Then there are $C < \infty$ and $\varepsilon_0 > 0$ such that for all $\varepsilon \leq \varepsilon_0, t \in \mathbb{R}$

$$\left\| \left(e^{-iH_{\mathcal{A}}^\varepsilon t} - A^* \mathcal{U}^{\varepsilon*} e^{-iH_{\text{eff}}^\varepsilon t} \mathcal{U}^\varepsilon A \right) A^* \mathcal{P}^\varepsilon \chi(H^\varepsilon) A \right\|_{\mathcal{L}(L^2(\mathcal{A}, d\tau))} < C \varepsilon^3 |t|$$

for each characteristic function χ with $\text{supp } \chi \subset (-\infty, E]$.

The proof of this result can be found in Section 3.2. Of course, the choice of our metric (10) changes the metric in a singular way because it blows up a region of finite volume to an infinite one. However, it will turn out that the image of \mathcal{P}^ε consists of functions that decay faster than any negative power of $|\zeta|/\varepsilon$ away from the zero section of the normal bundle. Therefore leaving the metric invariant on $\mathcal{B}_{\delta/2}$ is sufficient; due to the fast decay the error in the blown up region will be smaller than any power of ε for $\varepsilon \ll \delta$.

We note that the assumptions made about V^ε in Theorem 1 translate into local assumptions about $V_{\mathcal{A}}^\varepsilon$, i.e. they only have to be valid on a tubular neighborhood of \mathcal{C} with diameter of order δ . Furthermore $V^\varepsilon := AV_{\mathcal{A}}^\varepsilon A^*$ is convergent for $|\nu| \rightarrow \infty$. Therefore $H_{\text{f}}(q)$ has eigenvalues only below the continuous spectrum. Then a separated energy band is automatically a constraint energy band as was explained in the sequel to Definition 3.

2.2 The effective Hamiltonian

We write down the effective Hamiltonian only for states with high energies cut off. Then H_{eff} does not depend on any cutoff, which is a non-trivial fact, since we will need cutoffs to construct it!

Theorem 2 Let $\tilde{\psi}, \phi \in \overline{\mathcal{H}}$. In addition to the assumptions of Theorem 1 let $\varphi_0 \in C_b^\infty(\mathcal{C}, \mathcal{H}_f(q))$ be a global family of eigenfunctions corresponding to E_0 and $\tilde{\chi} \in C_0^\infty(\mathbb{R})$ with $\tilde{\chi}|_{[\inf \sigma(H^\varepsilon), E]} \equiv 1$ and $\text{supp } \tilde{\chi} \subset (-\infty, E + 1)$. For $\psi := \mathcal{U}\tilde{\chi}(H^\varepsilon)\mathcal{U}^*\chi(H_{\text{eff}}^\varepsilon)\tilde{\psi}$ the effective Hamiltonian $H_{\text{eff}}^\varepsilon$ from Theorem 1 is given, modulo terms of order $\varepsilon^3\|\phi\|\|\psi\|$, by

$$\begin{aligned} & \langle \phi | H_{\text{eff}}^\varepsilon \psi \rangle_{L^2(\mathcal{C}, d\mu_{\text{eff}}^\varepsilon)} \\ &= \int_{\mathcal{C}} \left(g_{\text{eff}}^\varepsilon((p_{\text{eff}}^\varepsilon \phi)^*, p_{\text{eff}}^\varepsilon \psi) + \phi^*(E_0 + \varepsilon \langle \varphi_0 | \nabla^\nu W \varphi_0 \rangle_{\mathcal{H}_f} + \varepsilon^2 W^{(2)}) \psi \right. \\ & \quad \left. - \varepsilon^2 \mathcal{M}(\Psi^*(\varepsilon \nabla p_{\text{eff}}^\varepsilon \phi, p_{\text{eff}}^\varepsilon \phi, \phi), \Psi(\varepsilon \nabla p_{\text{eff}}^\varepsilon \psi, p_{\text{eff}}^\varepsilon \psi, \psi)) \right) d\mu_{\text{eff}}^\varepsilon, \end{aligned}$$

where for $\tau_1, \tau_2 \in \Gamma(T^*\mathcal{C})$

$$\begin{aligned} g_{\text{eff}}^\varepsilon(\tau_1, \tau_2) &= g(\tau_1, \tau_2) + \varepsilon \langle \varphi_0 | 2\Pi(\cdot)(\tau_1, \tau_2) \varphi_0 \rangle_{\mathcal{H}_f} \\ & \quad + \varepsilon^2 \left\langle \varphi_0 \left| 3g(\mathcal{W}(\cdot)\tau_1, \mathcal{W}(\cdot)\tau_2) \varphi_0 + \overline{\mathcal{R}}(\tau_1, \cdot, \tau_2, \cdot) \varphi_0 \right. \right\rangle_{\mathcal{H}_f}, \\ p_{\text{eff}}^\varepsilon \psi &= -i \text{d}\psi - \left(\varepsilon i \langle \varphi_0 | \nabla^h \varphi_0 \rangle_{\mathcal{H}_f} + \varepsilon^2 i \int_{N_q \mathcal{C}} \frac{2}{3} \varphi_0^* \overline{\mathcal{R}}(\nabla^\nu \varphi_0, \nu) \nu d\nu \right. \\ & \quad \left. - \varepsilon^2 i \left\langle \varphi_0 \left| 2(\mathcal{W}(\cdot) - \langle \varphi_0 | \mathcal{W}(\cdot) \varphi_0 \rangle_{\mathcal{H}_f}) \nabla^h \varphi_0 \right. \right\rangle_{\mathcal{H}_f} \right) \psi, \end{aligned}$$

with \mathcal{W} the Weingarten mapping, Π the second fundamental form, $\overline{\mathcal{R}}$ the curvature mapping, $\overline{\mathcal{R}}$ the Riemann tensor, and $T_q^{(*)}\mathcal{C}$ and $N_q^{(*)}\mathcal{C}$ canonically included into $T_{(q,0)}^{(*)}N\mathcal{C}$. The arguments (\cdot) are integrated over the fibers.

Furthermore $W^{(2)} = \langle \varphi_0 | \frac{1}{2} \nabla^\nu \cdot W \varphi_0 \rangle_{\mathcal{H}_f} + V_{\text{BH}} + V_{\text{geom}} + V_{\text{amb}}$ and

$$\begin{aligned} V_{\text{BH}} &= \int_{N_q \mathcal{C}} g_{\text{eff}}^\varepsilon(\nabla^h \varphi_0^*, (1 - P_0) \nabla^h \varphi_0) d\nu, \\ V_{\text{geom}} &= -\frac{1}{4} \overline{g}(\eta, \eta) + \frac{1}{2} \kappa - \frac{1}{6} (\overline{\kappa} + \text{tr}_{\mathcal{C}} \overline{\text{Ric}} + \text{tr}_{\mathcal{C}} \overline{\mathcal{R}}), \\ V_{\text{amb}} &= \int_{N_q \mathcal{C}} \frac{1}{3} \overline{\mathcal{R}}(\nabla^\nu \varphi_0^*, \nu, \nabla^\nu \varphi_0, \nu) d\nu, \\ \mathcal{M}(\Phi, \Psi) &= \int_{N_q \mathcal{C}} \Phi (1 - P_0) (H_f - E_0)^{-1} (1 - P_0) \Psi d\nu, \\ \Psi(A, p, \phi) &= -\varphi_0 \text{tr}_{\mathcal{C}}(\mathcal{W}(\nu)A) - 2g_{\text{eff}}^\varepsilon(\nabla^h \varphi_0^*, p) + \varphi_0 V_1 \phi \end{aligned}$$

with η the mean curvature vector, $\kappa, \overline{\kappa}$ the scalar curvatures of \mathcal{C} and \mathcal{A} , and $\text{tr}_{\mathcal{C}} \overline{\text{Ric}}, \text{tr}_{\mathcal{C}} \overline{\mathcal{R}}$ the partial traces with respect to \mathcal{C} of the Ricci and the Riemann tensor of \mathcal{A} (see the appendix for definitions of all the geometric objects).

This result will be derived in Section 3.3. Some explanations of the numerous corrections and its consequences are in order.

Remark 2 *i) If \mathcal{C} is compact or contractible or if E_0 is the ground state energy of H_f , $V_0 \in C_b^\infty(\mathcal{C}, C_b^\infty(N_q\mathcal{C}))$ implies the extra assumption that $\varphi_0 \in C_b^\infty(\mathcal{C}, \mathcal{H}_f)$ (see Lemma 12 in Section 4.3). We do not know if this implication holds true in general.*

ii) The effective momentum $p_{\text{eff}}^\varepsilon$ induces a Berry connection (see Proposition 1 below). The first order correction in $p_{\text{eff}}^\varepsilon$ is the natural geometric generalization of the Berry term appearing in the Born-Oppenheimer setting (see [35]). The origin of the modification is the possible non-flatness of the normal bundle. When the constraining potential is not allowed to vary in shape but only to twist, the first-order correction reduces to the Berry term discussed by Mitchell in [23].

iii) The correction of the metric tensor by exterior curvature is a feature not realized before because tangential kinetic energies were taken to be small as a whole. Its origin is that the dynamics does not take place exactly on the submanifold. Therefore the mass distribution of the wavefunction in normal direction has to be accounted for when measuring distances.

iv) The off-band coupling \mathcal{M} and V_{BH} , an analogue of the so-called Born-Huang potential, also appear when adiabatic perturbation theory is applied to the Born-Oppenheimer setting. However, they are modified here if the curvature of the normal bundle does not vanish. Furthermore \mathcal{M} contains a new fourth order differential operator which comes from the exterior curvature. Both \mathcal{M} and V_{BH} can easily be checked to be gauge-invariant, i.e. not depending on φ_0 but only on P_0 .

v) The existence of the geometric extra potential V_{geom} has been stressed in the literature, in particular in the context of curvature-induced bound states (reviewed by Duclos and Exner in [11]). In our setting there are lots of situations when it is of minor importance because of the first order corrections. The potential V_{amb} was also found in [23].

We end this subsection with a closer look at the induced Berry connection.

Proposition 1 $\nabla_\tau^{\text{eff}}\psi := (ip_{\text{eff}}^\varepsilon\psi)(\tau)$ is a metric connection on the trivial complex line bundle over \mathcal{C} where ψ takes its values. Its curvature mapping is given by

$$\begin{aligned} R^{\nabla^{\text{eff}}}(\tau_1, \tau_2) &:= \nabla_{\tau_1}^{\text{eff}}\nabla_{\tau_2}^{\text{eff}} - \nabla_{\tau_2}^{\text{eff}}\nabla_{\tau_1}^{\text{eff}} - \nabla_{[\tau_1, \tau_2]}^{\text{eff}} \\ &= \varepsilon^2 \int_{N_q\mathcal{C}} \bar{g}(\varphi_0^* \nu, R^\perp(\tau_1, \tau_2)\nabla^\nu\varphi_0) d\nu + \mathcal{O}(\varepsilon^3), \end{aligned}$$

where R^\perp is the normal curvature mapping (defined in the appendix).

The proof is provided in Subsection 3.4. Although we consider a varying φ_0 , we obtain here the same expression for the curvature as Mitchell in [23]. The reason for this will turn out to be that φ_0 can be chosen to be real locally because H_f is real. In [23] the above expression is shown to vanish at all $q \in \mathcal{C}$ where $\varphi_0(q)$ has at least $k - 1$ distinct orthogonal axes of reflection symmetries. In [20] Maraner identifies it as the origin of roto-vibrational couplings in a simple molecular model.

3 Proof of the main results

In the following $\mathcal{D}(A)$ denotes the domain of an operator A . For convenience we set $\mathcal{D}(H^0) := \mathcal{H}$. We recall that we have set $\langle \nu \rangle := \sqrt{1 + |\nu|^2}$. $A = \langle \nu \rangle^l$ is meant to be the multiplication with $\langle \nu \rangle^l$. We write $a \lesssim b$ if a is bounded by b times a constant independent of ε , and $a = \mathcal{O}(\varepsilon^l)$ if $\|a\| \lesssim \varepsilon^l$. Finally we say that A is operator-bounded by B , $A \prec B$, if $\mathcal{D}(B) \subset \mathcal{D}(A)$ and $\|A\psi\| \lesssim \|B\psi\| + \|\psi\|$ for all $\psi \in \mathcal{D}(B)$.

3.1 Proof of adiabatic decoupling

As explained in the introduction the first step in proving adiabatic decoupling is the unitary transformation of H^ε by multiplication with the square root of the relative density $\rho := \frac{d\bar{\mu}}{d\mu \otimes d\nu}$ of the volume measure associated to \bar{g} and the product measure on $N\mathcal{C}$. The abstract statement reads as follows:

Lemma 1 *Let (\mathcal{M}, g) be a Riemannian manifold. Let $d\sigma_1, d\sigma_2$ be two measures on \mathcal{M} with smooth and positive relative density $\rho := \frac{d\sigma_1}{d\sigma_2}$. Define*

$$M_\rho : L^2(\mathcal{M}, d\sigma_1) \rightarrow L^2(\mathcal{M}, d\sigma_2), \psi \mapsto \rho^{\frac{1}{2}}\psi.$$

Then M_ρ is unitary and it holds

$$\begin{aligned} M_\rho(-\Delta_{d\sigma_1})M_\rho^*\psi &= -\Delta_{d\sigma_2}\psi - \left(\frac{1}{4}g(d(\ln \rho), d(\ln \rho)) - \frac{1}{2}\Delta_{d\tau}(\ln \rho)\right)\psi \\ &=: -\Delta_{d\sigma_2}\psi + V_\rho\psi, \end{aligned}$$

where $\Delta_{d\sigma_i} := \operatorname{div}_{d\sigma_i} \operatorname{grad} \psi$ and $\operatorname{div}_{d\sigma_i}$ is the adjoint of grad on $L^2(\mathcal{M}, d\sigma_i)$.

The proof is a simple calculation which can be found in the sequel to the proof of Theorem 1. We recall from (12) that $\rho = \frac{d\bar{\mu}}{d\mu \otimes d\nu}$ is in $C_b^\infty(N\mathcal{C})$ and strictly positive independently of ε . Therefore V_ρ is in $C_b^\infty(N\mathcal{C})$ for our choice of ρ . Since ρ is equal to 1 outside of $B_{\delta/2}$, V_ρ is even in $C_b^\infty(\mathcal{C}, C_b^\infty(N_q\mathcal{C}))$.

The heart of Theorem 1 is the existence of a subspace $P_\varepsilon \mathcal{H} \subset \mathcal{H}$ that can be mapped unitarily to $L^2(\mathcal{C}, d\mu)$ and is approximately invariant under the time evolution:

Lemma 2 *Under the assumptions of Theorem 1 there is $\varepsilon_0 > 0$ such that for all $\varepsilon < \varepsilon_0$ there is a closed subspace $P_\varepsilon \mathcal{H} \subset \mathcal{H}$ with corresponding orthogonal projection $P_\varepsilon \in \mathcal{L}(\mathcal{H})$ such that for each $m \in \mathbb{N}_0$ and $\chi \in C^\infty(\mathbb{R}, [0, 1])$ with $\text{supp } \chi \subset (-\infty, E + 1]$ it holds $P_\varepsilon \in \mathcal{L}(\mathcal{D}(H_\varepsilon^m))$ and*

$$\|[H_\varepsilon, P_\varepsilon]\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon), \mathcal{H})} = \mathcal{O}(\varepsilon), \quad \|[H_\varepsilon, P_\varepsilon] \chi(H_\varepsilon)\|_{\mathcal{L}(\mathcal{H}, \mathcal{D}(H_\varepsilon^m))} = \mathcal{O}(\varepsilon^3). \quad (20)$$

and

$$\forall j, l \in \mathbb{N}: \|\langle \nu \rangle^l P_\varepsilon \langle \nu \rangle^j\|_{\mathcal{L}(\mathcal{H})}, \|\langle \nu \rangle^l P_\varepsilon \langle \nu \rangle^j\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon))} \lesssim 1. \quad (21)$$

Furthermore there is a unitary \tilde{U}_ε with $P_\varepsilon = \tilde{U}_\varepsilon^* P_0 \tilde{U}_\varepsilon$ and $\|\tilde{U}_\varepsilon - 1\|_{\mathcal{L}(\mathcal{H})} = \mathcal{O}(\varepsilon)$.

The construction of P_ε and \tilde{U}_ε is carried out in Section 4.3. When we take its existence for granted, it is not difficult to prove that the effective dynamics on the submanifold is a good approximation.

PROOF OF THEOREM 1 (SECTION 2.1):

Let $d\mu_{\text{eff}}^\varepsilon$ be the volume measure associated to $g_{\text{eff}}^\varepsilon$ which is given by the expression in Theorem 2. For any fixed $E < \infty$ Lemma 2 yields some unitary \tilde{U}_ε for all ε below a certain ε_0 . We define $U_\varepsilon := U_0 \tilde{U}_\varepsilon$. Using Remark 1 and Lemma 2 we have

$$U_\varepsilon^* U_\varepsilon = \tilde{U}_\varepsilon^* U_0^* U_0 U_\varepsilon = \tilde{U}_\varepsilon^* P_0 \tilde{U}_\varepsilon = P_\varepsilon.$$

In view of Lemma 1, we next set $\mathcal{U}^\varepsilon := M_{\tilde{\rho}} U_\varepsilon D_\varepsilon M_\rho$ with $\rho := \frac{d\bar{\mu}}{d\mu \otimes d\nu}$ and $\tilde{\rho} := \frac{d\mu}{d\mu_{\text{eff}}^\varepsilon}$. Furthermore we define $\mathcal{P}^\varepsilon := \mathcal{U}^{\varepsilon*} \mathcal{U}^\varepsilon$. Then, indeed, \mathcal{U}^ε is unitary from $\mathcal{P}^\varepsilon \mathcal{H}$ to $L^2(\mathcal{C}, d\mu_{\text{eff}}^\varepsilon)$. Finally we set

$$H_{\text{eff}}^\varepsilon := \mathcal{U}^\varepsilon H^\varepsilon \mathcal{U}^{\varepsilon*} = M_{\tilde{\rho}} U_\varepsilon H_\varepsilon U_\varepsilon^* M_{\tilde{\rho}}^*. \quad (22)$$

We notice that $H_{\text{eff}}^\varepsilon$ is symmetric by definition. U_ε is unitary when restricted to $P_\varepsilon \mathcal{H}$ due to Lemma 2. So the self-adjointness of $H_{\text{eff}}^\varepsilon$ is implied by the self-adjointness of $P_\varepsilon H_\varepsilon P_\varepsilon$, which is in turn a consequence of the self-adjointness of $P_\varepsilon H_\varepsilon P_\varepsilon + (1 - P_\varepsilon) H_\varepsilon (1 - P_\varepsilon)$. For ε small enough this last self-adjointness can be verified using Lemma 2 and the Kato-Rellich theorem (see [29]):

$$\begin{aligned} H_\varepsilon &- (P_\varepsilon H_\varepsilon P_\varepsilon + (1 - P_\varepsilon) H_\varepsilon (1 - P_\varepsilon)) \\ &= (1 - P_\varepsilon) H_\varepsilon P_\varepsilon + P_\varepsilon H_\varepsilon (1 - P_\varepsilon) \\ &= (1 - P_\varepsilon) [H_\varepsilon, P_\varepsilon] - P_\varepsilon [H_\varepsilon, P_\varepsilon] \\ &= (1 - 2P_\varepsilon) [H_\varepsilon, P_\varepsilon]. \end{aligned}$$

Lemma 2 entails that $[H_\varepsilon, P_\varepsilon]$ is operator-bounded by $\varepsilon H_\varepsilon$. Hence, for ε small enough (we adjust ε_0 if necessary) the difference above is operator-bounded by H_ε with relative bound smaller than one. Now the Kato-Rellich theorem yields the claim, because H_ε is self-adjoint (as it is unitarily equivalent to the selfadjoint H^ε).

In order to check that (19) is an immediate consequence of (18) it suffices to verify that $\|\mathcal{U}^\varepsilon - \mathcal{U}_0^\varepsilon\|_{\mathcal{L}(\overline{\mathcal{H}}, L^2(\mathcal{C}, d\mu_{\text{eff}}^\varepsilon))} = \mathcal{O}(\varepsilon)$. Since $\|\tilde{U}_\varepsilon - 1\|_{\mathcal{L}(\mathcal{H})} = \mathcal{O}(\varepsilon)$ by Lemma 2 and $\|\tilde{\rho} - 1\|_\infty = \mathcal{O}(\varepsilon)$ by definition of $d\mu_{\text{eff}}^\varepsilon$, we obtain that

$$\begin{aligned} \|\mathcal{U}^\varepsilon - \mathcal{U}_0^\varepsilon\|_{\mathcal{L}(\overline{\mathcal{H}}, L^2(\mathcal{C}, d\mu_{\text{eff}}^\varepsilon))} &= \|M_{\tilde{\rho}} U_0 P_0 \tilde{U}_\varepsilon D_\varepsilon M_\rho - U_0 P_0 D_\varepsilon\|_{\mathcal{L}(\overline{\mathcal{H}}, L^2(\mathcal{C}, d\mu_{\text{eff}}^\varepsilon))} \\ &= \|U_0 P_0 D_\varepsilon (M_\rho - 1)\|_{\mathcal{L}(\overline{\mathcal{H}}, L^2(\mathcal{C}, d\mu))} + \mathcal{O}(\varepsilon) \\ &\lesssim \|\langle \nu \rangle^{-1} D_\varepsilon (M_\rho - 1)\|_{\mathcal{L}(\overline{\mathcal{H}}, \mathcal{H})} + \mathcal{O}(\varepsilon), \end{aligned}$$

where we used $\|P_0 \langle \nu \rangle\|_{\mathcal{L}(\mathcal{H})} \lesssim 1$ in the last step. In view of (12) a first order Taylor expansion of M_ρ in normal directions yields that $D_\varepsilon (M_\rho - 1)$ is globally bounded by a constant times $\varepsilon \langle \nu \rangle$. So we end up with the desired estimate.

We now turn to the derivation of the estimate (18). To do so we first pull out the unitaries $M_{\tilde{\rho}}, M_\rho$ and D_ε . For the rest of the proof we drop the ε -subscripts of P_ε and U_ε .

$$\begin{aligned} &(e^{-iH^\varepsilon t} - \mathcal{U}^{\varepsilon*} e^{-iH_{\text{eff}} t} \mathcal{U}^\varepsilon) \mathcal{P}^\varepsilon \chi(H^\varepsilon) \\ &= M_\rho^* D_\varepsilon^* (e^{-iD_\varepsilon M_\rho H^\varepsilon M_\rho^* D_\varepsilon^* t} - U^* e^{-iM_{\tilde{\rho}} H_{\text{eff}} M_{\tilde{\rho}}^* t} U) D_\varepsilon M_\rho \mathcal{P}^\varepsilon \chi(H^\varepsilon) \\ &= M_\rho^* D_\varepsilon^* (e^{-iH_\varepsilon t} - U^* e^{-iUH_\varepsilon U^* t} U) D_\varepsilon M_\rho \mathcal{U}^{\varepsilon*} \mathcal{U}^\varepsilon \chi(H^\varepsilon) \\ &= M_\rho^* D_\varepsilon^* (e^{-iH_\varepsilon t} - U^* e^{-iUH_\varepsilon U^* t} U) U^* M_{\tilde{\rho}}^* M_{\tilde{\rho}} U D_\varepsilon M_\rho \chi(H^\varepsilon) \\ &= M_\rho^* D_\varepsilon^* (e^{-iH_\varepsilon t} - U^* e^{-iUH_\varepsilon U^* t} U) U^* U \chi(H_\varepsilon) D_\varepsilon M_\rho \end{aligned}$$

Since M_ρ and D_ε are unitary, we can ignore them for the estimate and continue with the term in the middle. Next we use Duhamel's principle to express the difference of the unitary groups as a difference of its generators. Because of $UU^* = 1$ and $P = U^*U$ we have that

$$\begin{aligned} &(e^{-iH_\varepsilon t} - U^* e^{-iUH_\varepsilon U^* t} U) U^* U \chi(H_\varepsilon) \\ &= (P - U^* e^{-iUH_\varepsilon U^* t} U e^{iH_\varepsilon t}) e^{-iH_\varepsilon t} \chi(H_\varepsilon) + [e^{-iH_\varepsilon t}, P] \chi(H_\varepsilon) \\ &= i \int_0^t U^* e^{-iUH_\varepsilon U^* s} (UH_\varepsilon U^* U - UH_\varepsilon) e^{iH_\varepsilon s} \chi(H_\varepsilon) ds e^{-iH_\varepsilon t} \\ &\quad + [e^{-iH_\varepsilon t}, P] \chi(H_\varepsilon) \\ &\stackrel{(22)}{=} i \int_0^t U^* e^{-iUH_\varepsilon U^* s} U (H_\varepsilon P - PH_\varepsilon) \chi(H_\varepsilon) e^{iH_\varepsilon s} ds e^{-iH_\varepsilon t} \\ &\quad + [e^{-iH_\varepsilon t}, P] \chi(H_\varepsilon). \quad (23) \end{aligned}$$

Now we observe that $[H_\varepsilon, P] \chi(H_\varepsilon) = [H_\varepsilon, U^*U] \chi(H_\varepsilon) = \mathcal{O}(\varepsilon^3)$ implies that

$$\| [e^{-iH_\varepsilon t}, P] \chi(H_\varepsilon) \|_{\mathcal{L}(\mathcal{H})} = \mathcal{O}(\varepsilon^3 |t|), \quad (24)$$

since $[e^{-iH_\varepsilon t}, \chi(H_\varepsilon)] = 0$ due to the spectral theorem and

$$\begin{aligned} [e^{-iH_\varepsilon t}, P] \chi(H_\varepsilon) &= e^{-iH_\varepsilon t} (P - e^{iH_\varepsilon t} P e^{-iH_\varepsilon t}) \chi(H_\varepsilon) \\ &= -e^{-iH_\varepsilon t} i \int_0^t e^{iH_\varepsilon s} (H_\varepsilon P - P H_\varepsilon) e^{-iH_\varepsilon s} ds \chi(H_\varepsilon) \\ &= -e^{-iH_\varepsilon t} i \int_0^t e^{iH_\varepsilon s} [H_\varepsilon, P] \chi(H_\varepsilon) e^{-iH_\varepsilon s} ds. \end{aligned}$$

So in view of (23)

$$\begin{aligned} &\| (e^{-iH_\varepsilon t} - U^* e^{-iUH_\varepsilon U^* t} U) P \chi(H_\varepsilon) \|_{\mathcal{L}(\mathcal{H})} \\ &\stackrel{(24)}{\leq} \left\| \int_0^t U^* e^{-iUH_\varepsilon U^* s} U (H_\varepsilon P - P H_\varepsilon) \chi(H_\varepsilon) e^{iH_\varepsilon s} ds \right\|_{\mathcal{L}(\mathcal{H})} + \mathcal{O}(\varepsilon^3 |t|) \\ &\leq t \underbrace{\| U^* e^{-iUH_\varepsilon U^* s} U \|_{\mathcal{L}(\mathcal{H})}}_{\leq 1} \| [H_\varepsilon, P] \chi(H_\varepsilon) \|_{\mathcal{L}(\mathcal{H})} \underbrace{\| e^{iH_\varepsilon s} \|_{\mathcal{L}(\mathcal{H})}}_{=1} + \mathcal{O}(\varepsilon^3 |t|) \\ &\stackrel{(20)}{=} \mathcal{O}(\varepsilon^3 |t|). \end{aligned}$$

by Lemma 2. This proves the error estimate (18). \square

PROOF OF LEMMA 1:

M_ρ is an isometry because for all $\psi, \varphi \in L^2(\mathcal{M}, d\sigma_1)$

$$\int_{\mathcal{M}} M_\rho \psi^* M_\rho \varphi d\sigma_2 = \int_{\mathcal{M}} \psi^* \varphi \rho d\sigma_2 = \int_{\mathcal{M}} \bar{\psi} \varphi d\sigma_1.$$

Therefore it is clear that

$$M_\rho^* \psi = \rho^{-\frac{1}{2}} \psi$$

which is well-defined since ρ is positive. One immediately concludes

$$M_\rho M_\rho^* = \text{Id} = M_\rho^* M_\rho$$

and thus M_ρ is unitary. Now we note that $[\text{grad}, \rho^{-\frac{1}{2}}] = -\frac{1}{2} \rho^{-\frac{1}{2}} \text{grad} \ln \rho$. So we have

$$\begin{aligned} M_\rho(-\Delta_{d\sigma_1}) M_\rho^* \psi &= -\rho^{\frac{1}{2}} \text{div}_{d\sigma_1} \text{grad}(\rho^{-\frac{1}{2}} \psi) \\ &= -\rho^{\frac{1}{2}} \text{div}_{d\sigma_1} \rho^{-\frac{1}{2}} (\text{grad} \psi - \frac{1}{2} (\text{grad} \ln \rho) \psi) \\ &= -\rho^{\frac{1}{2}} \text{div}_{d\sigma_1} \rho^{-\frac{1}{2}} \text{grad} \psi + \rho^{\frac{1}{2}} \text{div}_{d\sigma_1} \left(\rho^{-\frac{1}{2}} \frac{1}{2} (\text{grad} \ln \rho) \psi \right) \end{aligned}$$

On the one hand

$$\rho^{\frac{1}{2}} \operatorname{div}_{d\sigma_1} \rho^{-\frac{1}{2}} \operatorname{grad} \psi = \rho \operatorname{div}_{d\sigma_1} \rho^{-1} \operatorname{grad} \psi + \frac{1}{2} g(\operatorname{grad} \ln \rho, \operatorname{grad} \psi)$$

and on the other hand

$$\begin{aligned} \rho^{\frac{1}{2}} \operatorname{div}_{d\sigma_1} \left(\rho^{-\frac{1}{2}} \frac{1}{2} (\operatorname{grad} \ln \rho) \psi \right) &= -\frac{1}{4} g(\operatorname{grad} \ln \rho, \operatorname{grad} \ln \rho) \psi \\ &\quad + \frac{1}{2} \operatorname{div}_{d\sigma_1} (\operatorname{grad} \ln \rho) \psi \\ &\quad + \frac{1}{2} g(\operatorname{grad} \ln \rho, \operatorname{grad} \psi). \end{aligned}$$

Together we obtain

$$\begin{aligned} M_\rho(-\Delta_{d\sigma_1})M_\rho^* \psi &= -\rho \operatorname{div}_{d\sigma_1} \rho^{-1} \operatorname{grad} \psi \\ &\quad - \left(\frac{1}{4} g(\operatorname{grad} \ln \rho, \operatorname{grad} \ln \rho) - \frac{1}{2} \operatorname{div}_{d\sigma_1} \operatorname{grad} \ln \rho \right) \psi \\ &= -\Delta_{d\sigma_2} \psi - \left(\frac{1}{4} g(\operatorname{grad} \ln \rho, \operatorname{grad} \ln \rho) - \frac{1}{2} \Delta_{d\sigma_1} \ln \rho \right) \psi, \end{aligned}$$

which is the claim. \square

3.2 Pullback of the results to the ambient space

First we state an immediate consequence of Lemma 2 for the projector \mathcal{P}^ε that was defined at the beginning of the proof of Theorem 1.

Corollary 2 *For each $\chi \in C^\infty(\mathbb{R}, [0, 1])$ with $\operatorname{supp} \chi \subset (-\infty, E + 1]$ it holds $\mathcal{P}^\varepsilon \in \mathcal{L}(\overline{\mathcal{H}}) \cap \mathcal{L}(\mathcal{D}(H^\varepsilon))$ and*

$$\| [H^\varepsilon, \mathcal{P}^\varepsilon] \|_{\mathcal{L}(\mathcal{D}(H^\varepsilon), \overline{\mathcal{H}})} = \mathcal{O}(\varepsilon), \quad \| [H^\varepsilon, \mathcal{P}^\varepsilon] \chi(H^\varepsilon) \|_{\mathcal{L}(\overline{\mathcal{H}})} = \mathcal{O}(\varepsilon^3). \quad (25)$$

Furthermore

$$\forall l, m \in \mathbb{N} : \| \langle \nu / \varepsilon \rangle^l \mathcal{P}^\varepsilon \langle \nu / \varepsilon \rangle^m \|_{\mathcal{L}(\overline{\mathcal{H}})}, \| \langle \nu / \varepsilon \rangle^l \mathcal{P}^\varepsilon \langle \nu / \varepsilon \rangle^m \|_{\mathcal{L}(\mathcal{D}(H^\varepsilon))} \lesssim 1. \quad (26)$$

We omit the proof which uses only the unitarity of M_ρ and D_ε as well as $D_\varepsilon \langle \nu \rangle D_\varepsilon^* = \langle \nu / \varepsilon \rangle$. Now we gather some facts about the operator A defined in (4) and its adjoint.

Lemma 3 *Let A be defined by $A\psi := \frac{d\bar{\mu}}{\Phi^* d\tau} (\psi \circ \Phi)$ with $\Phi : \mathcal{NC} \rightarrow \mathcal{B}_\delta$ as constructed in Section 1.1.*

i) It holds $A \in \mathcal{L}(L^2(\mathcal{A}, d\tau), \overline{\mathcal{H}})$ with

$$\| A\psi \|_{L^2(\mathcal{NC}, d\bar{\mu})} \leq \| \psi \|_{L^2(\mathcal{A}, d\tau)} \quad \forall \psi \in L^2(\mathcal{A}, d\tau).$$

ii) For $\varphi \in \overline{\mathcal{H}}$ the adjoint A^* of A is given by

$$A^* \varphi = \begin{cases} \left(\frac{\Phi^* d\tau}{d\bar{\mu}} \varphi \right) \circ \Phi^{-1} & \text{on } \mathcal{B}_\delta, \\ 0 & \text{on } \mathcal{A} \setminus \mathcal{B}_\delta. \end{cases}$$

It satisfies $\|A^* \varphi\|_{L^2(\mathcal{A}, d\tau)} = \|\varphi\|_{L^2(N\mathcal{C}, d\bar{\mu})}$, $A^* A = \chi_{\mathcal{B}_\delta}$, and $AA^* = 1$.

iii) $A^* \mathcal{P}_\varepsilon \in \mathcal{L}(\mathcal{D}(H^\varepsilon), \mathcal{D}(H_{\mathcal{A}}^\varepsilon))$ and

$$\|(H_{\mathcal{A}}^\varepsilon A^* - A^* H^\varepsilon) \mathcal{P}^\varepsilon\|_{\mathcal{L}(\mathcal{D}(H^\varepsilon), L^2(\mathcal{A}, d\tau))} \lesssim \varepsilon^3. \quad (27)$$

The last estimate is crucial for the proof of Corollary 1. It results from the two facts that $H_{\mathcal{A}} A^* = A^* H^\varepsilon$ on $\mathcal{B}_{\delta/2}$ by construction and that \mathcal{P}^ε is small on the complement. Lemma 3 will be proved at the end of Section 4.1. We now turn to the short derivation of Corollary 1.

PROOF OF COROLLARY 1 (SECTION 2.1):

By Lemma 3 we have $AA^* = 1$. Therefore

$$\begin{aligned} & (e^{-iH_{\mathcal{A}}^\varepsilon t} - A^* \mathcal{U}^{\varepsilon*} e^{-iH_{\text{eff}}^\varepsilon t} \mathcal{U}^\varepsilon A) A^* \mathcal{P}^\varepsilon \chi(H^\varepsilon) A \\ &= \left((e^{-iH_{\mathcal{A}}^\varepsilon t} A^* - A^* e^{-iH^\varepsilon t}) + A^* (e^{-iH^\varepsilon t} - \mathcal{U}^{\varepsilon*} e^{-iH_{\text{eff}}^\varepsilon t} \mathcal{U}^\varepsilon) \right) \mathcal{P}^\varepsilon \chi(H^\varepsilon) A \end{aligned}$$

Since A and A^* are bounded by Lemma 3, Theorem 1 implies that the second difference is of order $\varepsilon^3|t|$. So it suffices to estimate the first difference. The estimate (25) implies $[e^{-iH^\varepsilon t}, \mathcal{P}^\varepsilon] \chi(H^\varepsilon) = \mathcal{O}(\varepsilon^3|t|)$ analogously with the proof of (24). So

$$\begin{aligned} & (e^{-iH_{\mathcal{A}}^\varepsilon t} A^* - A^* e^{-iH^\varepsilon t}) \mathcal{P}^\varepsilon \chi(H^\varepsilon) A \\ &= e^{-iH_{\mathcal{A}}^\varepsilon t} (A^* \mathcal{P}^\varepsilon - e^{iH_{\mathcal{A}}^\varepsilon t} A^* \mathcal{P}^\varepsilon e^{-iH^\varepsilon t}) \chi(H^\varepsilon) A + A^* [e^{-iH^\varepsilon t}, \mathcal{P}^\varepsilon] \chi(H^\varepsilon) A \\ &= ie^{-iH_{\mathcal{A}}^\varepsilon t} \int_0^t e^{iH_{\mathcal{A}}^\varepsilon s} (A^* \mathcal{P}^\varepsilon H^\varepsilon - H_{\mathcal{A}}^\varepsilon A^* \mathcal{P}^\varepsilon) e^{iH_{\mathcal{A}}^\varepsilon s} \chi(H^\varepsilon) A ds + \mathcal{O}(\varepsilon^3|t|) \\ &= ie^{-iH_{\mathcal{A}}^\varepsilon t} \int_0^t e^{iH_{\mathcal{A}}^\varepsilon s} (A^* H^\varepsilon - H_{\mathcal{A}}^\varepsilon A^*) \mathcal{P}^\varepsilon \chi(H^\varepsilon) e^{iH_{\mathcal{A}}^\varepsilon s} A ds + \mathcal{O}(\varepsilon^3|t|) \\ &= \mathcal{O}(\varepsilon^3|t|) \end{aligned}$$

due to (27) and $\chi(H^\varepsilon) \in \mathcal{L}(L^2(N\mathcal{C}, d\bar{\mu}), \mathcal{D}(H^\varepsilon))$. \square

3.3 Derivation of the effective Hamiltonian

The Hamiltonian can be expanded with respect to the normal directions when operating on functions that decay fast enough. To do so we split up the integration over $N\mathcal{C}$ into an integration over the fibers $N_q\mathcal{C}$, isomorphic to \mathbb{R}^k , followed by an integration over \mathcal{C} , which is always possible for a measure of the form $d\mu \otimes d\nu$ (see chapter XVI, §4 of [18]).

Lemma 4 *Let $m \in \mathbb{N}_0$. If a densely defined operator P satisfies*

$$\|P\langle\nu\rangle^l\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon^m), \mathcal{H})} \lesssim 1, \quad \|\langle\nu\rangle^l P\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon^{m+1}), \mathcal{D}(H_\varepsilon))} \lesssim 1$$

for every $l \in \mathbb{N}$, then the operators $H_\varepsilon P, PH_\varepsilon \in \mathcal{L}(\mathcal{D}(H_\varepsilon^{m+1}), \mathcal{H})$ can be expanded in powers of ε in the sense of bounded operators:

$$\begin{aligned} H_\varepsilon P &= (H_0 + \varepsilon H_1 + \varepsilon^2 H_2) P + \mathcal{O}(\varepsilon^3), \\ P H_\varepsilon &= P (H_0 + \varepsilon H_1 + \varepsilon^2 H_2) + \mathcal{O}(\varepsilon^3) \end{aligned}$$

where H_0, H_1, H_2 are the operators associated with

$$\begin{aligned} \langle\phi|H_0\psi\rangle_{\mathcal{H}} &= \int_{\mathcal{C}} \int_{N_q\mathcal{C}} g(\varepsilon\nabla^h\phi^*, \varepsilon\nabla^h\psi) d\nu d\mu + \langle\phi|H_f\psi\rangle_{\mathcal{H}}, \\ \langle\phi|H_1\psi\rangle_{\mathcal{H}} &= \int_{\mathcal{C}} \int_{N_q\mathcal{C}} 2\Pi_\nu(\varepsilon\nabla^h\phi^*, \varepsilon\nabla^h\psi) + \phi^* \nabla_\nu^v W \psi d\nu d\mu, \\ \langle\phi|H_2\psi\rangle_{\mathcal{H}} &= \int_{\mathcal{C}} \int_{N_q\mathcal{C}} 3g(\mathcal{W}_\nu \varepsilon\nabla^h\phi^*, \mathcal{W}_\nu \varepsilon\nabla^h\psi) + \mathcal{R}(\varepsilon\nabla^h\phi^*, \nu, \varepsilon\nabla^h\psi, \nu) \\ &\quad + \frac{2}{3}\mathcal{R}(\varepsilon\nabla^h\phi^*, \nu, \nabla^v\psi, \nu) + \frac{2}{3}\mathcal{R}(\nabla^v\phi^*, \nu, \varepsilon\nabla^h\psi, \nu) \\ &\quad + \frac{1}{3}\mathcal{R}(\nabla^v\phi^*, \nu, \nabla^v\psi, \nu) + \phi^* (\frac{1}{2}\nabla_{\nu,\nu}^v W + V_{\text{geom}})\psi d\nu d\mu. \end{aligned} \tag{28}$$

Furthermore for $l = 0, 1, 2$

$$H_l P \prec H_\varepsilon^{m+1}, \quad P H_l \prec H_\varepsilon^{m+1}. \tag{29}$$

This will be proven in Section 4.2. Definition 3 and Lemma 2 imply that Lemma 4 can be applied to the relevant projectors P_0 and P_ε with $m = 0$. In the next lemma we gather some useful properties of P_0 , the global family of associated eigenfunctions φ_0 (see Remark 1), and \tilde{U}_ε (see Lemma 2):

Lemma 5 *It holds*

- i) $\forall l, m \in \mathbb{N}_0$: $\|\langle\nu\rangle^l P_0 \langle\nu\rangle^m\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon))} \lesssim 1$, $\|[-\varepsilon^2 \Delta_h, P_0]\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon), \mathcal{H})} \lesssim \varepsilon$.*
- ii) There are $U_1^\varepsilon, U_2^\varepsilon \in \mathcal{L}(\mathcal{H}) \cap \mathcal{L}(\mathcal{D}(H_\varepsilon))$ with norms bounded independently of ε satisfying $P_0 U_1^\varepsilon P_0 = 0$ and $U_2^\varepsilon P_0 = P_0 U_2^\varepsilon P_0 = P_0 U_2^\varepsilon$ such that $\tilde{U}_\varepsilon = 1 + \varepsilon U_1^\varepsilon + \varepsilon^2 U_2^\varepsilon$.*
- iii) $\|P_0 U_1^\varepsilon \langle\nu\rangle^l\|_{\mathcal{L}(\mathcal{H})} \lesssim 1$ for all $l \in \mathbb{N}_0$.*
- iv) For $B^\varepsilon := U_0^* U_\varepsilon \chi(H_\varepsilon)$ and all $u \in \{1, (U_1^\varepsilon)^*, (U_2^\varepsilon)^*\}$ it holds*

$$\|[-\varepsilon^2 \Delta_h + E_0, u P_0] B^\varepsilon\|_{\mathcal{L}(\mathcal{H})} = \mathcal{O}(\varepsilon). \tag{30}$$

v) For $R_{H_f}(E_0) := (1 - P_0)(H_f - E_0)^{-1}(1 - P_0)$ it holds

$$\|U_1^{\varepsilon*} B^\varepsilon + R_{H_f}(E_0) ([-\varepsilon \Delta_h, P_0] + H_1) P_0 B^\varepsilon\|_{\mathcal{L}(\mathcal{H}, \mathcal{D}(H_\varepsilon))} = \mathcal{O}(\varepsilon) \quad (31)$$

vi) If $\varphi_0 \in C_b^m(\mathcal{C}, \mathcal{H}_f)$, there is $\lambda_0 \gtrsim 1$ with $\sup_q \|e^{\lambda_0 \langle \nu \rangle} \varphi_0(q)\|_{\mathcal{H}_f(q)} \lesssim 1$ and

$$\sup_{q \in \mathcal{C}} \|e^{\lambda_0 \langle \nu \rangle} \nabla_{\nu_1, \dots, \nu_l}^v \nabla_{\tau_1, \dots, \tau_m}^h \varphi_0(q)\|_{\mathcal{H}_f(q)} \lesssim 1$$

for all $\nu_1, \dots, \nu_l \in \Gamma_b(N\mathcal{C})$ and $\tau_1, \dots, \tau_m \in \Gamma_b(T\mathcal{C})$.

Since U_2^ε does only effect $P_\varepsilon \mathcal{H}$ but not the effective Hamiltonian, we have not stated its particular form here. The proof of this lemma can be found in Section 4.3. To calculate the effective Hamiltonian we also need the following commutator estimates.

Lemma 6 Let $\chi_1 \in C_0^\infty(\mathbb{R})$, $(H, \mathcal{D}(H))$ be selfadjoint on \mathcal{H} , and $A \in \mathcal{L}(\mathcal{H})$.

a) Let $\chi_2 : \mathbb{R} \rightarrow \mathbb{R}$ be a bounded Borel function. If there are $j, l, m \in \mathbb{N}$ with $\|[H, A] \chi_2(H)\|_{\mathcal{L}(\mathcal{D}(H^l), \mathcal{D}(H^{m-1}))} \lesssim \varepsilon^j$, then

$$\|[\chi_1(H), A] \chi_2(H)\|_{\mathcal{L}(\mathcal{D}(H^{l-1}), \mathcal{D}(H^m))} \lesssim \varepsilon^j.$$

b) Let $B \in \mathcal{L}(\mathcal{H}, \tilde{\mathcal{H}})$ with $BB^* = 1$ and $B^*B = A$. Assume that the operator $(\tilde{H} := BHB^*, \mathcal{D}(\tilde{H}))$ is selfadjoint on $\tilde{\mathcal{H}}$. If there is $j \in \mathbb{N}_0$ such that $\|[H, A]\|_{\mathcal{L}(\mathcal{D}(H), \mathcal{H})} \leq \varepsilon^j$, then

$$\|\chi_1(\tilde{H}) - B\chi_1(H)B^*\|_{\mathcal{L}(\tilde{\mathcal{H}}, \mathcal{D}(\tilde{H}))} \lesssim \varepsilon^{2j}.$$

These statements can be generalized in many ways. Here we have given versions which are sufficient for the situations that we encounter in the following. We emphasize that the support of χ_2 need not be compact, in particular $\chi_2 \equiv 1$ is allowed. Now we are ready to derive the effective Hamiltonian. Lemma 6 will be proved afterwards.

PROOF OF THEOREM 2 (SECTION 2.2):

We recall that we defined $U_\varepsilon := U_0 \tilde{U}_\varepsilon$, $\mathcal{U}^\varepsilon := M_{\tilde{\rho}} U_\varepsilon M_\rho$, $\mathcal{P}^\varepsilon := \mathcal{U}^{\varepsilon*} \mathcal{U}^\varepsilon$, and $H_{\text{eff}}^\varepsilon := \mathcal{U}^\varepsilon H^\varepsilon \mathcal{U}^{\varepsilon*}$ in the Proof of Theorem 1, which implied $P_\varepsilon = U_\varepsilon^* U_\varepsilon$.

By Theorem 1 $H_{\text{eff}}^\varepsilon$ is selfadjoint. Furthermore $\mathcal{U}^\varepsilon \mathcal{U}^{\varepsilon*} = U_0 U_0^* = 1$. So, in view of Corollary 2, \mathcal{P}^ε and \mathcal{U}^ε satisfy the assumptions on A and B in Lemma 6 with $j = 1$. Let χ and $\tilde{\chi} \in C_0^\infty(\mathbb{R})$ as in the theorem. Then the spectral calculus for selfadjoint operators implies $\tilde{\chi}(H_{\text{eff}}^\varepsilon) \chi(H_{\text{eff}}^\varepsilon) = \chi(H_{\text{eff}}^\varepsilon)$.

Therefore

$$\begin{aligned}
\|\chi(H_{\text{eff}}^\varepsilon)\tilde{\psi}\| &= \|\tilde{\chi}(H_{\text{eff}}^\varepsilon)\chi(H_{\text{eff}}^\varepsilon)\tilde{\psi}\| \\
&\lesssim \|\mathcal{U}^\varepsilon\tilde{\chi}(H^\varepsilon)\mathcal{U}^{\varepsilon*}\chi(H_{\text{eff}}^\varepsilon)\tilde{\psi}\| + \varepsilon^2\|\chi(H_{\text{eff}}^\varepsilon)\tilde{\psi}\| \\
&= \|\psi\| + \varepsilon^2\|\chi(H_{\text{eff}}^\varepsilon)\tilde{\psi}\|.
\end{aligned}$$

For ε small enough this implies $\|\chi(H_{\text{eff}}^\varepsilon)\tilde{\psi}\| \lesssim \|\psi\|$. Hence, it is enough to prove estimates by $\|\chi(H_{\text{eff}}^\varepsilon)\tilde{\psi}\|$.

For arbitrary ψ we set $\psi_{\tilde{\rho}} := M_{\tilde{\rho}}^*\psi$. In the sequel we omit the ε -scripts of U_1^ε , U_2^ε , and \tilde{U}_ε . We claim that

$$\begin{aligned}
\langle \phi | H_{\text{eff}} \psi \rangle &= \langle \phi_{\tilde{\rho}} | M_{\tilde{\rho}}^* H_{\text{eff}} M_{\tilde{\rho}} \psi_{\tilde{\rho}} \rangle \\
&= \langle \phi_{\tilde{\rho}} | U H_\varepsilon U^* \psi_{\tilde{\rho}} \rangle \\
&= \langle \phi_{\tilde{\rho}} | U_0 (H_0 + \varepsilon H_1 + \varepsilon^2 H_2) U_0^* \psi_{\tilde{\rho}} \rangle \\
&\quad + \varepsilon \langle \phi_{\tilde{\rho}} | U_0 (U_1 (H_0 + \varepsilon H_1) + (H_0 + \varepsilon H_1) U_1^*) U_0^* \psi_{\tilde{\rho}} \rangle \\
&\quad + \varepsilon^2 \langle \phi_{\tilde{\rho}} | U_0 (U_1 H_0 U_1^* + U_2 H_0 + H_0 U_2^*) U_0^* \psi_{\tilde{\rho}} \rangle \\
&\quad + \mathcal{O}(\varepsilon^3 \|\phi\| \|\psi\|). \tag{32}
\end{aligned}$$

If we could just count the number of ε 's after plugging in the expansion from Lemma 4 for H_ε and the one from Lemma 5 for \tilde{U} , this would be clear. But the expansion of H_ε yields polynomially growing coefficients. So we have to use carefully the estimate (29) which is allowed due to the decay properties of P , P_0 , and $P_0 U_1$ from Lemma 2 and Lemma 5.

In view of Lemma 2 P_ε satisfies the assumptions on P in Lemma 4 for $m = 0$ and thus $\|P_\varepsilon(H_\varepsilon - (H_0 + \varepsilon H_1 + \varepsilon^2 H_2))\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon), \mathcal{H})} = \mathcal{O}(\varepsilon^3)$. We notice that $\chi(H_\varepsilon) \in \mathcal{L}(\mathcal{H}, \mathcal{D}(H_\varepsilon))$ because H_ε is bounded from below and the support of χ is bounded from above. By Lemma 5 it holds $u \in \mathcal{L}(\mathcal{D}(H_\varepsilon))$ for each $u \in \{\tilde{U}^*, 1, U_1^*, U_2^*\}$. Furthermore Lemma 5 implies that $u P_0$ satisfies the assumptions on P in Lemma 4 for all such u because $\tilde{U}^* P_0 = P_\varepsilon \tilde{U}^* P_0$ and $U_2^* P_0 = P_0 U_2^* P_0$. Hence, we may conclude from (29) that

$$\|h u U_0^* \psi_{\tilde{\rho}}\| = \|h u P_0 \tilde{U} \chi(H_\varepsilon) U^* (\chi(H_{\text{eff}}^\varepsilon)\tilde{\psi})_{\tilde{\rho}}\| \lesssim \|\chi(H_{\text{eff}}^\varepsilon)\tilde{\psi}\| \tag{33}$$

for each $h \in \{H_\varepsilon, H_0, H_1, H_2\}$. So, recalling that $\|\chi(H_{\text{eff}}^\varepsilon)\tilde{\psi}\|$ is estimated by $\|\psi\|$ we have

$$\begin{aligned}
U H_\varepsilon U^* \psi_{\tilde{\rho}} &= U P_\varepsilon H_\varepsilon \tilde{U}^* U_0^* \psi_{\tilde{\rho}} \\
&= U P_\varepsilon (H_0 + \varepsilon H_1 + \varepsilon^2 H_2) \tilde{U}^* U_0^* \psi_{\tilde{\rho}} + \mathcal{O}(\varepsilon^3 \|\psi\|) \\
&= U P_\varepsilon (H_0 + \varepsilon H_1 + \varepsilon^2 H_2) (1 + \varepsilon U_1^* + \varepsilon^2 U_2^*) U_0^* \psi_{\tilde{\rho}} + \mathcal{O}(\varepsilon^3 \|\psi\|) \\
&= U \left((H_0 + \varepsilon H_1 + \varepsilon^2 H_2) \right. \\
&\quad \left. + \varepsilon (H_0 + \varepsilon H_1) U_1^* + \varepsilon^2 H_0 U_2^* \right) U_0^* \psi_{\tilde{\rho}} + \mathcal{O}(\varepsilon^3 \|\psi\|).
\end{aligned}$$

For the rest of the proof we write $\mathcal{O}(\varepsilon^l)$ for bounded by $\varepsilon^l \|\phi\| \|\psi\|$ times a constant independent of ε . Using that $U_0^* = P_0 U_0^*$ and $P_0 U_2 = U_2 P_0$ by Lemma 5 we obtain

$$\begin{aligned} \langle \phi | H_{\text{eff}} \psi \rangle &= \langle \phi_{\bar{\rho}} | U H_{\varepsilon} U^* \psi_{\bar{\rho}} \rangle \\ &= \langle \phi_{\bar{\rho}} | U (H_0 + \varepsilon H_1 + \varepsilon^2 H_2) P_0 U_0^* \psi_{\bar{\rho}} \rangle \\ &\quad + \varepsilon \langle \phi_{\bar{\rho}} | U (H_0 + \varepsilon H_1) U_1^* P_0 U_0^* \psi_{\bar{\rho}} \rangle \\ &\quad + \varepsilon^2 \langle U_0^* \phi_{\bar{\rho}} | U H_0 P_0 U_2 U_0^* \psi_{\bar{\rho}} \rangle + \mathcal{O}(\varepsilon^3), \end{aligned} \quad (34)$$

After plugging $U = (1 + \varepsilon U_1 + \varepsilon^2 U_2) U_0^*$ we may drop the terms with three or more ε 's in it because of (33). Gathering all the remaining terms we, indeed, end up with (32).

Now we set $\mathcal{H}_s := L^2(\mathcal{C}, d\mu)$ and calculate all the terms in (32) separately. Remark 1 yields that for any operator A

$$\langle \phi_{\bar{\rho}} | U_0 A U_0^* \psi_{\bar{\rho}} \rangle_{\mathcal{H}_s} = \langle \varphi_0 \phi_{\bar{\rho}} | A \varphi_0 \psi_{\bar{\rho}} \rangle_{\mathcal{H}}. \quad (35)$$

In view of Definition 1 we have

$$\begin{aligned} \nabla^v \psi_{\bar{\rho}} \varphi_0 &= \psi_{\bar{\rho}} \nabla^v \varphi_0, \\ \varepsilon \nabla^h \psi_{\bar{\rho}} \varphi_0 &= \varphi_0 \varepsilon d\psi_{\bar{\rho}} + \psi_{\bar{\rho}} \varepsilon \nabla^h \varphi_0, \end{aligned}$$

where d is the exterior derivative on \mathcal{C} . We note that $\sup_q \|\varepsilon \nabla^h \varphi_0\|_{\mathcal{H}_t(q)}$ is of order ε by Lemma 5. Furthermore the exponential decay of φ_0 and its derivatives due to the same Lemma guarantees that in the sequel all the ν -integrals are bounded in spite of the terms growing polynomially in ν . These facts will be used throughout the computations below. We write them as quadratic forms for the sake of readability. However, one should think of all the operators applied to ϕ as the adjoint applied to the corresponding term containing ψ . We have

$$\begin{aligned} &\langle \varphi_0 \phi_{\bar{\rho}} | H_0 \varphi_0 \psi_{\bar{\rho}} \rangle_{\mathcal{H}} \\ &\stackrel{(28)}{=} \int_{\mathcal{C}} \phi_{\bar{\rho}}^* \langle \varphi_0 | H_{\text{f}} \varphi_0 \rangle_{\mathcal{H}_{\text{f}}} \psi_{\bar{\rho}} d\mu + \int_{\mathcal{C}} \int_{N_q \mathcal{C}} g(\varepsilon \nabla^h \varphi_0^* \phi_{\bar{\rho}}^*, \varepsilon \nabla^h \varphi_0 \psi_{\bar{\rho}}) d\nu d\mu \\ &= \int_{\mathcal{C}} \phi_{\bar{\rho}}^* E_0 \psi_{\bar{\rho}} d\mu + \int_{\mathcal{C}} \int_{N_q \mathcal{C}} |\varphi_0|^2 g(\varepsilon d\phi_{\bar{\rho}}^*, \varepsilon d\psi_{\bar{\rho}}) + \varepsilon g(\varphi_0^* \varepsilon d\phi_{\bar{\rho}}^*, \psi_{\bar{\rho}} \nabla^h \varphi_0) \\ &\quad + \varepsilon g(\phi_{\bar{\rho}}^* \nabla^h \varphi_0^*, \varphi_0 \varepsilon d\psi_{\bar{\rho}}) + \varepsilon^2 g(\phi_{\bar{\rho}}^* \nabla^h \varphi_0^*, \psi_{\bar{\rho}} \nabla^h \varphi_0) d\nu d\mu \\ &= \int_{\mathcal{C}} g((p_{\text{eff}} \phi_{\bar{\rho}})^*, p_{\text{eff}} \psi_{\bar{\rho}}) + \phi_{\bar{\rho}}^* E_0 \psi_{\bar{\rho}} + \varepsilon^2 \phi_{\bar{\rho}}^* V_{\text{BH}} \psi_{\bar{\rho}} d\mu \\ &\quad - \varepsilon^2 \int_{\mathcal{C}} g(\varepsilon d\phi_{\bar{\rho}}^*, \psi_{\bar{\rho}} (R_1 + R_2)) + g(\phi_{\bar{\rho}}^* (R_1 + R_2), \varepsilon d\psi_{\bar{\rho}}) d\mu \end{aligned} \quad (36)$$

with remainder terms $R_1 := \langle \varphi_0 | 2(\mathcal{W}(\cdot) - \langle \varphi_0 | \mathcal{W}(\cdot) \varphi_0 \rangle_{\mathcal{H}_f}) \nabla^h \varphi_0 \rangle_{\mathcal{H}_f}$ and $R_2 := \int_{N_q \mathcal{C}} \frac{2}{3} \varphi_0^* \mathbb{R}(\nabla^v \varphi_0, \nu) \nu d\nu$. R_1 is cancelled by a term coming from H_1 :

$$\begin{aligned}
& \langle \varphi_0 \phi_{\bar{\rho}} | H_1 \varphi_0 \psi_{\bar{\rho}} \rangle_{\mathcal{H}} \\
& \stackrel{(28)}{=} \int_{\mathcal{C}} \int_{N_q \mathcal{C}} 2\Pi(\nu) (\varepsilon \nabla^h \varphi_0^* \phi_{\bar{\rho}}^*, \varepsilon \nabla^h \varphi_0 \psi_{\bar{\rho}}) + \phi_{\bar{\rho}}^* (\nabla_\nu^v W) |\varphi_0|^2 \psi_{\bar{\rho}} d\nu d\mu \\
& = \int_{\mathcal{C}} \int_{N_q \mathcal{C}} |\varphi_0|^2 2\Pi(\nu) (\varepsilon d\phi_{\bar{\rho}}^*, \varepsilon d\psi_{\bar{\rho}}) + \varepsilon 2\Pi(\nu) (\varphi_0^* \varepsilon d\phi_{\bar{\rho}}^*, \psi_{\bar{\rho}} \nabla^h \varphi_0) \\
& \quad + \varepsilon 2\Pi(\nu) (\phi_{\bar{\rho}}^* \nabla^h \varphi_0^*, \varphi_0 \varepsilon d\psi_{\bar{\rho}}) + \phi_{\bar{\rho}}^* (\nabla_\nu^v W) |\varphi_0|^2 \psi_{\bar{\rho}} d\nu d\mu + \mathcal{O}(\varepsilon^2) \\
& = \int_{\mathcal{C}} \langle \varphi_0 | 2\Pi(\cdot) ((p_{\text{eff}} \phi_{\bar{\rho}})^*, p_{\text{eff}} \psi_{\bar{\rho}}) \varphi_0 \rangle_{\mathcal{H}_f} d\mu + \int_{\mathcal{C}} \phi_{\bar{\rho}}^* \langle \varphi_0 | (\nabla^v W) \varphi_0 \rangle_{\mathcal{H}_f} \psi_{\bar{\rho}} d\mu \\
& \quad + \varepsilon \int_{\mathcal{C}} g(\varepsilon d\phi_{\bar{\rho}}^*, \psi_{\bar{\rho}} R_1) + g(\phi_{\bar{\rho}}^* R_1, \varepsilon d\psi_{\bar{\rho}}) d\mu + \mathcal{O}(\varepsilon^2). \tag{37}
\end{aligned}$$

At second order we first omit the terms involving the Riemann tensor:

$$\begin{aligned}
& \langle \varphi_0 \phi_{\bar{\rho}} | H_2 \varphi_0 \psi_{\bar{\rho}} \rangle_{\mathcal{H}} - \text{'Riemann-terms'} \\
& \stackrel{(28)}{=} \int_{\mathcal{C}} \int_{N_q \mathcal{C}} 3g(\mathcal{W}(\nu) \varepsilon \nabla^h \varphi_0^* \phi_{\bar{\rho}}^*, \mathcal{W}(\nu) \varepsilon \nabla^h \varphi_0 \psi_{\bar{\rho}}) \\
& \quad + \phi_{\bar{\rho}}^* (\frac{1}{2} \nabla_{\nu, \nu}^v W + V_{\text{geom}}) |\varphi_0|^2 \psi_{\bar{\rho}} d\nu d\mu \\
& = \int_{\mathcal{C}} \langle \varphi_0 | 3g(\mathcal{W}(\cdot) \varepsilon d\phi_{\bar{\rho}}^*, \mathcal{W}(\cdot) \varepsilon d\psi_{\bar{\rho}}) \varphi_0 \rangle_{\mathcal{H}_f} d\mu + \mathcal{O}(\varepsilon) \\
& \quad + \int_{\mathcal{C}} \phi_{\bar{\rho}}^* (\langle \varphi_0 | (\frac{1}{2} \nabla_{\cdot, \cdot}^v W) \varphi_0 \rangle_{\mathcal{H}_f} + V_{\text{geom}}) \psi_{\bar{\rho}} d\mu \\
& = \int_{\mathcal{C}} \langle \varphi_0 | 3g(\mathcal{W}(\cdot) (p_{\text{eff}} \psi_{\bar{\rho}})^*, \mathcal{W}(\cdot) p_{\text{eff}} \psi_{\bar{\rho}}) \varphi_0 \rangle_{\mathcal{H}_f} d\mu \\
& \quad + \int_{\mathcal{C}} \phi_{\bar{\rho}}^* (\langle \varphi_0 | (\frac{1}{2} \nabla_{\cdot, \cdot}^v W) \varphi_0 \rangle_{\mathcal{H}_f} + V_{\text{geom}}) \psi_{\bar{\rho}} d\mu + \mathcal{O}(\varepsilon), \tag{38}
\end{aligned}$$

where we used that $i\varepsilon d\psi_{\bar{\rho}} - p_{\text{eff}}\psi_{\bar{\rho}} = \mathcal{O}(\varepsilon)$ in the last step. Now we take care of the omitted second order terms.

'Riemann-terms'

$$\begin{aligned}
&\stackrel{(28)}{=} \int_{\mathcal{C}} \int_{N_q \mathcal{C}} \overline{\mathcal{R}}(\varepsilon \nabla^h \varphi_0^* \phi_{\bar{\rho}}^*, \nu, \varepsilon \nabla^h \varphi_0 \psi_{\bar{\rho}}, \nu) + \frac{2}{3} \overline{\mathcal{R}}(\varepsilon \nabla^h \varphi_0^* \phi_{\bar{\rho}}^*, \nu, \nabla^v \varphi_0 \psi_{\bar{\rho}}, \nu) \\
&\quad + \frac{2}{3} \overline{\mathcal{R}}(\nabla^v \varphi_0^* \phi_{\bar{\rho}}^*, \nu, \varepsilon \nabla^h \varphi_0 \psi_{\bar{\rho}}, \nu) + \frac{1}{3} \overline{\mathcal{R}}(\nabla^v \varphi_0^* \phi_{\bar{\rho}}^*, \nu, \nabla^v \varphi_0 \psi_{\bar{\rho}}, \nu) d\nu d\mu \\
&= \int_{\mathcal{C}} \int_{N_q \mathcal{C}} |\varphi_0|^2 \overline{\mathcal{R}}(\varepsilon d\phi_{\bar{\rho}}^*, \nu, \varepsilon d\psi_{\bar{\rho}}, \nu) + \frac{2}{3} \overline{\mathcal{R}}(\varphi_0^* \varepsilon d\phi_{\bar{\rho}}^*, \nu, \psi_{\bar{\rho}} \nabla^v \varphi_0, \nu) \\
&\quad + \frac{2}{3} \overline{\mathcal{R}}(\phi_{\bar{\rho}}^* \nabla^v \varphi_0^*, \nu, \varphi_0 \varepsilon d\psi_{\bar{\rho}}, \nu) + \frac{1}{3} \phi_{\bar{\rho}}^* \overline{\mathcal{R}}(\nabla^v \varphi_0^*, \nu, \nabla^v \varphi_0, \nu) \psi_{\bar{\rho}} d\nu d\mu + \mathcal{O}(\varepsilon) \\
&= \int_{\mathcal{C}} \langle \varphi_0 | \overline{\mathcal{R}}(\varepsilon d\phi_{\bar{\rho}}^*, \cdot, \varepsilon d\psi_{\bar{\rho}}, \cdot) \varphi_0 \rangle_{\mathcal{H}_f} d\mu + \int_{\mathcal{C}} \phi_{\bar{\rho}}^* V_{\text{amb}} \psi_{\bar{\rho}} d\mu \\
&\quad + \int_{\mathcal{C}} g(\phi_{\bar{\rho}}^* R_2, \varepsilon d\psi_{\bar{\rho}}) + g(\varepsilon d\phi_{\bar{\rho}}^*, \psi_{\bar{\rho}} R_2) d\mu + \mathcal{O}(\varepsilon). \tag{39}
\end{aligned}$$

Again replacing $i\varepsilon d\psi_{\bar{\rho}}$ with $p_{\text{eff}}\psi_{\bar{\rho}}$ and g with g_{eff} yields errors of order ε only. In view of (35)-(39), we have

$$\begin{aligned}
&\langle \phi_{\bar{\rho}} | U_0 (H_0 + \varepsilon H_1 + \varepsilon^2 H_2) U_0^* \psi_{\bar{\rho}} \rangle_{\mathcal{H}_s} \\
&= \int_{\mathcal{C}} g_{\text{eff}}^{\varepsilon}((p_{\text{eff}}\phi_{\bar{\rho}})^*, p_{\text{eff}}\psi_{\bar{\rho}}) + \phi_{\bar{\rho}}^* E_0 \psi_{\bar{\rho}} \\
&\quad + \phi_{\bar{\rho}}^* (\varepsilon \langle \varphi_0 | \nabla^v W \varphi_0 \rangle_{\mathcal{H}_f} + \varepsilon^2 W^{(2)}) \psi_{\bar{\rho}} d\mu + \mathcal{O}(\varepsilon^3). \tag{40}
\end{aligned}$$

Before we deal with the corrections by U_1 and U_2 we notice that due to $(1 - P_0)U_0^* = 0$ and $U_0 U_0^* = 1$

$$\begin{aligned}
&(1 - P_0)([-\varepsilon \Delta_h, P_0] + H_1) U_0^* \psi_{\bar{\rho}} \\
&= (1 - P_0)([-\varepsilon \Delta_h, U_0^* U_0] - \text{tr}_{\mathcal{C}} \varepsilon \nabla^h \mathcal{W}(\nu) \varepsilon \nabla^h + V_1) U_0^* \psi_{\bar{\rho}} \\
&= (1 - P_0)(V_1 - \text{tr}_{\mathcal{C}}(2(\nabla^h \varphi_0)U_0 + \varepsilon \nabla^h \mathcal{W}(\nu)) \varepsilon \nabla^h) U_0^* \psi_{\bar{\rho}} + \mathcal{O}(\varepsilon) \\
&= (1 - P_0)(\varphi_0 V_1 \psi_{\bar{\rho}} - 2g(\nabla^h \varphi_0^*, \varepsilon d\psi_{\bar{\rho}}) - \varphi_0 \text{tr}_{\mathcal{C}}(\mathcal{W}(\nu) \varepsilon^2 \nabla d\psi_{\bar{\rho}})) + \mathcal{O}(\varepsilon) \\
&= (1 - P_0)(\varphi_0 V_1 \psi_{\bar{\rho}} - \varphi_0 \text{tr}_{\mathcal{C}}(\mathcal{W}(\nu) \varepsilon^2 \nabla d\psi_{\bar{\rho}}) - 2g_{\text{eff}}^{\varepsilon}(\nabla^h \varphi_0^*, \varepsilon d\psi_{\bar{\rho}})) + \mathcal{O}(\varepsilon) \\
&= (1 - P_0) \Psi(\varepsilon^2 \nabla d\psi_{\bar{\rho}}, \varepsilon d\psi_{\bar{\rho}}, \psi_{\bar{\rho}}) + \mathcal{O}(\varepsilon). \tag{41}
\end{aligned}$$

We note that $U_0^* \psi_{\bar{\rho}} = BU^*(\chi(H_{\text{eff}})\tilde{\psi})_{\bar{\rho}}$. So we may apply (30) und (31) in the following. Since $U_0 = U_0 P_0$ by definition and we know from Lemma 5 that $P_0 U_1 P_0 = 0$, the first corrections by U_1 are an order of ε higher than

expected:

$$\begin{aligned}
& \left\langle \phi_{\bar{\rho}} \left| U_0 \left((H_0 + \varepsilon H_1) U_1^* + U_1 (H_0 + \varepsilon H_1) \right) U_0^* \psi_{\bar{\rho}} \right\rangle_{\mathcal{H}_s} \\
&= \left\langle \phi_{\bar{\rho}} \left| U_0 \left(([P_0, H_0] + \varepsilon H_1) U_1^* + U_1 ([H_0, P_0] + \varepsilon H_1) \right) U_0^* \psi_{\bar{\rho}} \right\rangle_{\mathcal{H}_s} \\
&= \varepsilon \left\langle \phi_{\bar{\rho}} \left| U_0 \left(([\varepsilon \Delta_h, P_0] + H_1) U_1^* + U_1 ([-\varepsilon \Delta_h, P_0] + H_1) P_0 \right) U_0^* \psi_{\bar{\rho}} \right\rangle_{\mathcal{H}_s} \\
&\stackrel{(31)}{=} -\varepsilon \left\langle \phi_{\bar{\rho}} \left| U_0 \left(([\varepsilon \Delta_h, P_0] + H_1) R_{H_f}(E_0) ([-\varepsilon \Delta_h, P_0] + H_1) U_0^* \psi_{\bar{\rho}} \right) \right\rangle_{\mathcal{H}_s} \\
&\quad - \varepsilon \left\langle \phi_{\bar{\rho}} \left| U_0 U_1 (H_f - E_0) U_1^* U_0^* \psi_{\bar{\rho}} \right\rangle_{\mathcal{H}_s} \\
&\stackrel{(41)}{=} -\varepsilon \left\langle \Psi(\varepsilon^2 \nabla d\phi_{\bar{\rho}}, \varepsilon d\phi_{\bar{\rho}}, \phi_{\bar{\rho}}) \left| R_{H_f}(E_0) \Psi(\varepsilon^2 \nabla d\psi_{\bar{\rho}}, \varepsilon d\psi_{\bar{\rho}}, \psi_{\bar{\rho}}) \right\rangle_{\mathcal{H}_s} \\
&\quad - \varepsilon \left\langle \phi_{\bar{\rho}} \left| U_0 U_1 (H_f - E_0) U_1^* U_0^* \psi_{\bar{\rho}} \right\rangle_{\mathcal{H}_s} \\
&= -\varepsilon \int_{\mathcal{C}} \mathcal{M}(\Psi^*(\varepsilon^2 \nabla d\phi_{\bar{\rho}}, \varepsilon d\phi_{\bar{\rho}}, \phi_{\bar{\rho}}), \Psi(\varepsilon^2 \nabla d\psi_{\bar{\rho}}, \varepsilon d\psi_{\bar{\rho}}, \psi_{\bar{\rho}})) d\mu \\
&\quad - \varepsilon \left\langle \phi_{\bar{\rho}} \left| U_0 U_1 (H_f - E_0) U_1^* U_0^* \psi_{\bar{\rho}} \right\rangle_{\mathcal{H}_s}. \tag{42}
\end{aligned}$$

Furthermore

$$\begin{aligned}
& \left\langle \phi_{\bar{\rho}} \left| U_0 (U_2 H_0 + H_0 U_2^*) U_0^* \psi_{\bar{\rho}} \right\rangle_{\mathcal{H}_s} \\
&= \left\langle U_0^* \phi_{\bar{\rho}} \left| P_0 (U_2 (-\varepsilon^2 \Delta_h + H_f) + (-\varepsilon^2 \Delta_h + H_f) U_2^*) P_0 U_0^* \psi_{\bar{\rho}} \right\rangle_{\mathcal{H}_s} \\
&= \left\langle U_0^* \phi_{\bar{\rho}} \left| (P_0 U_2 (-\varepsilon^2 \Delta_h + E_0) P_0 + P_0 (-\varepsilon^2 \Delta_h + E_0) U_2^* P_0) U_0^* \psi_{\bar{\rho}} \right\rangle_{\mathcal{H}_s} \\
&\stackrel{(30)}{=} \left\langle U_0^* \phi_{\bar{\rho}} \left| P_0 (U_2 + U_2^*) P_0 (-\varepsilon^2 \Delta_h + E_0) U_0^* \psi_{\bar{\rho}} \right\rangle_{\mathcal{H}_s} + \mathcal{O}(\varepsilon) \\
&= -\left\langle U_0^* \phi_{\bar{\rho}} \left| P_0 U_1 U_1^* P_0 (-\varepsilon^2 \Delta_h + E_0) U_0^* \psi_{\bar{\rho}} \right\rangle_{\mathcal{H}_s} + \mathcal{O}(\varepsilon), \tag{43}
\end{aligned}$$

since $\tilde{U} = 1 + \varepsilon U_1 + \varepsilon^2 U_2$ implies via $P_0 \tilde{U} \tilde{U}^* P_0 = P_0$ and $P_0 U_1 P_0 = 0$ that $P_0 (U_2 + U_2^*) P_0 = -P_0 U_1 U_1^* P_0 + \mathcal{O}(\varepsilon)$. Finally the remaining second order term cancels the term from (43) and the second term from (42):

$$\begin{aligned}
& \left\langle \phi_{\bar{\rho}} \left| U_0 U_1 H_0 U_1^* U_0^* \psi_{\bar{\rho}} \right\rangle_{\mathcal{H}_s} \\
&= \left\langle \phi_{\bar{\rho}} \left| U_0 U_1 (-\varepsilon^2 \Delta_h + H_f) U_1^* U_0^* \psi_{\bar{\rho}} \right\rangle_{\mathcal{H}_s} \\
&= \left\langle \phi_{\bar{\rho}} \left| U_0 U_1 (H_f - E_0) U_1^* U_0^* \psi_{\bar{\rho}} + U_0 U_1 (-\varepsilon^2 \Delta_h + E_0) U_1^* P_0 U_0^* \psi_{\bar{\rho}} \right\rangle_{\mathcal{H}_s} \\
&\stackrel{(30)}{=} \left\langle \phi_{\bar{\rho}} \left| U_0 U_1 (H_f - E_0) U_1^* U_0^* \psi_{\bar{\rho}} \right\rangle_{\mathcal{H}_s} \\
&\quad + \left\langle \phi_{\bar{\rho}} \left| U_0 U_1 U_1^* P_0 (-\varepsilon^2 \Delta_h + E_0) U_0^* \psi_{\bar{\rho}} \right\rangle_{\mathcal{H}_s} + \mathcal{O}(\varepsilon). \tag{44}
\end{aligned}$$

We gather the terms from (40) to (43) and replace $d\psi_{\bar{\rho}}$ by $p_{\text{eff}}^\varepsilon \psi_{\bar{\rho}}$ in the argument of Ψ , which only yields an error of order ε^3 . Then we almost obtain the claimed expression for the quadratic form of H_{eff} , only with $d\mu$ instead of $d\mu_{\text{eff}}$. Here $M_{\bar{\rho}}$ comes into play. By Lemma 1 the unitary transformation $M_{\bar{\rho}}$

interchanges the former with the latter and adds an extra potential. Verifying that this potential is only of order ε^3 finishes the proof. It is given by

$$-\frac{1}{4}g(\varepsilon d(\ln \tilde{\rho}), \varepsilon d(\ln \tilde{\rho})) + \frac{1}{2}\varepsilon^2 \Delta_{d\mu}(\ln \tilde{\rho}).$$

So it suffices to show that derivatives of $\ln \tilde{\rho}$ are of order ε . But this is clear: g and g_{eff} coincide at leading order and so do their associated volume measures. Therefore $d(\ln \tilde{\rho})$'s leading order term vanishes. \square

PROOF OF LEMMA 6:

We want to apply the so called Helffer-Sjöstrand formula (see [7], chapter 2) to χ_1 . It states that for any $\chi \in C_0^\infty(\mathbb{R})$

$$\chi(H) = \frac{1}{\pi} \int_{\mathbb{C}} \partial_{\bar{z}} \tilde{\chi}(z) R_H(z) dz, \quad (45)$$

where $R_H(z) := (H - z)^{-1}$ denotes the resolvent and $\tilde{\chi} : \mathbb{C} \rightarrow \mathbb{C}$ is a so-called almost analytic extension of χ . We emphasize that by dz we mean the usual volume on \mathbb{C} . With $z = x + iy$ a possible choice for $\tilde{\chi}$ is

$$\tilde{\chi}(x + iy) := \tau(y) \sum_{j=0}^l \chi^{(j)}(x) \frac{(iy)^j}{j!}$$

with arbitrary $\tau \in C^\infty(\mathbb{R}, [0, 1])$ satisfying $\tau|_{[-1, 1]} \equiv 1$ and $\text{supp } \tau \subset [-2, 2]$ and $l \geq 2$. Then obviously $\tilde{\chi} = \chi$ for $y = 0$ and

$$\partial_{\bar{z}} \tilde{\chi}(z) := \partial_x \tilde{\chi} + i \partial_y \tilde{\chi} = \mathcal{O}(|\text{Im} z|^l), \quad (46)$$

which is the reason why it is called an almost analytic extension. We choose such an almost analytic continuation $\tilde{\chi}_1 \in C_0^\infty(\mathbb{C})$ of χ_1 with $l = 2$. Next we observe that for all $j \in \mathbb{N}_0$

$$\|R_H(z)\|_{\mathcal{L}(\mathcal{D}(H^j), \mathcal{D}(H^{j+1}))} \leq \frac{\sqrt{1 + 2|\text{Im} z|^2 + 2|z|^2}}{|\text{Im} z|} \quad (47)$$

because for all $\psi \in \mathcal{H}$

$$\begin{aligned} \|H^{j+1} R_H(z) \psi\|^2 + \|R_H(z) \psi\|^2 &= \|H R_H(z) H^j \psi\|^2 + \|R_H(z) \psi\|^2 \\ &\leq \|(1 + z R_H(z)) H^j \psi\|^2 + \|R_H(z) \psi\|^2 \\ &\leq \left(2 + \frac{2|z|^2}{|\text{Im} z|^2}\right) \|H^j \psi\|^2 + \frac{1}{|\text{Im} z|^2} \|\psi\|^2 \\ &\leq \frac{1 + 2|\text{Im} z|^2 + 2|z|^2}{|\text{Im} z|^2} (\|\psi\|^2 + \|H^j \psi\|^2). \end{aligned}$$

Now by the Helffer-Sjöstrand formula

$$\begin{aligned}
[\chi_1(H), A] \chi_2(H) &= \frac{1}{\pi} \int_{\mathbb{C}} \partial_{\bar{z}} \tilde{\chi}_1(z) [R_H(z), A] dz \chi_2(H) \\
&= \frac{1}{\pi} \int_{\mathbb{C}} \partial_{\bar{z}} \tilde{\chi}_1(z) R_H(z) [A, H] R_H(z) dz \chi_2(H) \\
&= \frac{1}{\pi} \int_{\mathbb{C}} \partial_{\bar{z}} \tilde{\chi}_1(z) R_H(z) [A, H] \chi_2(H) R_H(z) dz,
\end{aligned}$$

where we used that $[R_H(z), \chi_2(H)] = 0$ in the last step. Using the assumption $\| [A, H] \chi_2(H) \|_{\mathcal{L}(\mathcal{D}(H^l), \mathcal{D}(H^m))} \leq \varepsilon^j$ we obtain

$$\begin{aligned}
&\| [\chi_1(H), A] \chi_2(H) \|_{\mathcal{L}(\mathcal{D}(H^{l-1}), \mathcal{D}(H^{m+1}))} \\
&\leq \frac{1}{\pi} \int_{\mathbb{C}} |\partial_{\bar{z}} \tilde{\chi}_1(z)| \| R_H(z) \|_{\mathcal{L}(\mathcal{D}(H^m), \mathcal{D}(H^{m+1}))} \\
&\quad \times \| [H, A] \chi_2(H) \|_{\mathcal{L}(\mathcal{D}(H^l), \mathcal{D}(H^m))} \| R_H(z) \|_{\mathcal{L}(\mathcal{D}(H^{l-1}), \mathcal{D}(H^l))} dz \\
&\stackrel{(46), (47)}{\lesssim} \varepsilon^j \int_{\text{supp } \tilde{\chi}_1} |\text{Im}z|^2 \frac{1 + 2|\text{Im}z|^2 + 2|z|^2}{|\text{Im}z|^2} dz \\
&\lesssim \varepsilon^j,
\end{aligned}$$

because χ_1 has compact support. This shows a).

The starting point for b) is the following observation:

$$\chi_1(\tilde{H}) - B\chi_1(H)B^* = \frac{1}{\pi} \int_{\mathbb{C}} \partial_{\bar{z}} \tilde{\chi}_1(z) (R_{\tilde{H}}(z) - BR_H(z)B^*) dz. \quad (48)$$

So we have to estimate $R_{\tilde{H}}(z) - BR_H(z)B^*$. We note that $B^*B = A$ and $BB^* = 1$ imply that $BA = B$, $AB^* = B^*$ and $A^2 = A$. By definition $\tilde{H} = BHB^*$. Therefore

$$\begin{aligned}
R_{\tilde{H}}(z) - BR_H(z)B^* &= R_{BHB^*}(z) (1 - (BHB^* - z)BR_H(z)B^*) \\
&= R_{\tilde{H}}(z) (1 - B(H - z)AR_H(z)B^*) \\
&= R_{\tilde{H}}(z) (1 - BAB^* - B[H, A]R_H(z)B^*) \\
&= -R_{\tilde{H}}(z) B[H, A]R_H(z)B^*.
\end{aligned}$$

Using that $A^2 = A$ entails $A[H, A]A = 0$ we get that

$$\begin{aligned}
R_{\tilde{H}}(z) - BR_H(z)B^* &= -R_{\tilde{H}}(z) BA[H, A](1 - A)R_H(z)AB^* \\
&= -R_{\tilde{H}}(z) BA[H, A](1 - A)[R_H(z), A]B^* \\
&= R_{\tilde{H}}(z) BA[H, A]R_H(z)[H, A]R_H(z)B^* \\
&= R_{\tilde{H}}(z) B[H, A]R_H(z)[H, A]R_H(z)B^*.
\end{aligned}$$

We note that (47) holds true with H replaced by \tilde{H} because \tilde{H} is assumed to be selfadjoint. Hence, we obtain

$$\begin{aligned}
& \|R_{\tilde{H}}(z) - BR_H(z)B^*\|_{\mathcal{L}(\tilde{\mathcal{H}}, \mathcal{D}(\tilde{H}))} \\
&= \|R_{\tilde{H}}(z)B[H, A]R_H(z)[H, A]R_H(z)B^*\|_{\mathcal{L}(\tilde{\mathcal{H}}, \mathcal{D}(\tilde{H}))} \\
&\lesssim \frac{\sqrt{1 + 2|\operatorname{Im}z|^2 + 2|z|^2}}{|\operatorname{Im}z|} \| [H, A] \|_{\mathcal{L}(\mathcal{D}(H), \mathcal{H})}^2 \|R_H(z)\|_{\mathcal{L}(\mathcal{H}, \mathcal{D}(H))}^2 \\
&\lesssim \varepsilon^{2j} \frac{(1 + 2|\operatorname{Im}z|^2 + 2|z|^2)^{3/2}}{|\operatorname{Im}z|^3}
\end{aligned}$$

by assumption. Together with (48) this yields the claim as in a) when we put $l = 3$ in the choice of the almost analytic extension. \square

3.4 Computation of the Berry connection's curvature

We will need that the (formal) connection ∇^h , which the normal connection induces on the bundle of functions over the normal fibers, is metric and the expression for its curvature.

Lemma 7 *It holds $\langle \nabla_\tau^h \phi | \psi \rangle_{\mathcal{H}_f} + \langle \phi | \nabla_\tau^h \psi \rangle_{\mathcal{H}_f} = (d\langle \phi | \psi \rangle_{\mathcal{H}_f})(\tau)$ and*

$$R^h(\tau_1, \tau_2)\psi := \left(\nabla_{\tau_1}^h \nabla_{\tau_2}^h - \nabla_{\tau_2}^h \nabla_{\tau_1}^h - \nabla_{[\tau_1, \tau_2]}^h \right) \psi = \bar{g}(\nu, R^\perp(\tau_1, \tau_2)\nabla^\nu \psi), \quad (49)$$

where R^\perp is the normal curvature mapping (defined in the appendix).

With this lemma we can compute the curvature of the effective Berry connection. The lemma itself will be proved afterwards.

PROOF OF PROPOSITION 1 (SECTION 2.2):

It is not difficult to verify that ∇^{eff} is indeed a connection. ∇^h is metric by Lemma 7 and so

$$2 \operatorname{Re} \langle \varphi_0 | \nabla^h \varphi_0 \rangle_{\mathcal{H}_f} = \langle \nabla_\tau^h \varphi_0 | \varphi_0 \rangle_{\mathcal{H}_f} + \langle \varphi_0 | \nabla_\tau^h \varphi_0 \rangle_{\mathcal{H}_f} = (d\langle \varphi_0 | \varphi_0 \rangle_{\mathcal{H}_f})(\tau) = 0.$$

Thus the correction in ∇^{eff} of order ε is purely imaginary. In a similar way it can be shown that the terms of order ε^2 are purely imaginary. Hence, for all $\psi_1, \psi_2 : \mathcal{C} \rightarrow \mathbb{C}$

$$\varepsilon d(\psi_1^* \psi_2)(\tau) = (\varepsilon d\psi_1^*)(\tau)\psi_2 + \psi_1^*(\varepsilon d\psi_2)(\tau) = (\nabla_\tau^{\text{eff}} \psi_1^*)\psi_2 + \psi_1^*(\nabla_\tau^{\text{eff}} \psi_2),$$

which means that ∇^{eff} is metric.

To compute the curvature we fix $q \in \mathcal{C}$ and choose again geodesic coordinate fields $\{\partial_{x_i}\}_{i=1,\dots,d}$ on an open neighbourhood Ω of q . Then $[\partial_{x_i}, \partial_{x_j}] = 0$ for all i, j . Implicitly summing over repeated indices we have

$$\begin{aligned}
\mathbb{R}^{\nabla^{\text{eff}}}(\tau_1, \tau_2)\psi &= (\nabla_{\tau_1}^{\text{eff}}\nabla_{\tau_2}^{\text{eff}} - \nabla_{\tau_2}^{\text{eff}}\nabla_{\tau_1}^{\text{eff}} - \nabla_{[\tau_1, \tau_2]}^{\text{eff}})\psi \\
&= \varepsilon^2 \tau_1^i \tau_2^j (\nabla_{\partial_{x_i}}^{\text{eff}}\nabla_{\partial_{x_j}}^{\text{eff}} - \nabla_{\partial_{x_j}}^{\text{eff}}\nabla_{\partial_{x_i}}^{\text{eff}})\psi \\
&= \varepsilon^2 \tau_1^i \tau_2^j (\partial_{x_i}\langle\varphi_0|\nabla_{\partial_{x_j}}^{\text{h}}\varphi_0\rangle - \partial_{x_j}\langle\varphi_0|\nabla_{\partial_{x_i}}^{\text{h}}\varphi_0\rangle)\psi + \mathcal{O}(\varepsilon^3) \\
&= \varepsilon^2 \tau_1^i \tau_2^j \left(\langle\varphi_0|\nabla_{\partial_{x_i}}^{\text{h}}\nabla_{\partial_{x_j}}^{\text{h}}\varphi_0\rangle + \langle\nabla_{\partial_{x_i}}^{\text{h}}\varphi_0|\nabla_{\partial_{x_j}}^{\text{h}}\varphi_0\rangle \right. \\
&\quad \left. - \langle\nabla_{\partial_{x_j}}^{\text{h}}\varphi_0|\nabla_{\partial_{x_i}}^{\text{h}}\varphi_0\rangle + \langle\varphi_0|\nabla_{\partial_{x_j}}^{\text{h}}\nabla_{\partial_{x_i}}^{\text{h}}\varphi_0\rangle \right)\psi + \mathcal{O}(\varepsilon^3),
\end{aligned}$$

where we used in the last step that ∇^{h} is metric again. Since H_f is real, we may choose a real family of φ_0 's on Ω . Then the second and the third term are equal and we obtain

$$\begin{aligned}
\mathbb{R}^{\nabla^{\text{eff}}}(\tau_1, \tau_2) &= \varepsilon^2 \tau_1^i \tau_2^j \langle\varphi_0|\nabla_{\partial_{x_i}}^{\text{h}}\nabla_{\partial_{x_j}}^{\text{h}}\varphi_0 - \nabla_{\partial_{x_j}}^{\text{h}}\nabla_{\partial_{x_i}}^{\text{h}}\varphi_0\rangle_{\mathcal{H}_f} + \mathcal{O}(\varepsilon^3) \\
&= \varepsilon^2 \langle\varphi_0|(\nabla_{\tau_1}^{\text{h}}\nabla_{\tau_2}^{\text{h}} - \nabla_{\tau_2}^{\text{h}}\nabla_{\tau_1}^{\text{h}} - \nabla_{[\tau_1, \tau_2]}^{\text{h}})\varphi_0\rangle_{\mathcal{H}_f} + \mathcal{O}(\varepsilon^3) \\
&= \varepsilon^2 \langle\varphi_0|\mathbb{R}^{\text{h}}(\tau_1, \tau_2)\varphi_0\rangle_{\mathcal{H}_f} + \mathcal{O}(\varepsilon^3) \\
&\stackrel{(49)}{=} \varepsilon^2 \int_{N_q\mathcal{C}} \bar{g}(\varphi_0^* \nu, \mathbb{R}^\perp(\tau_1, \tau_2)\nabla^{\text{v}}\varphi_0) d\nu + \mathcal{O}(\varepsilon^3),
\end{aligned}$$

which was to be shown. \square

PROOF OF LEMMA 7:

Again we fix $q \in \mathcal{C}$ and choose geodesic coordinate fields $\{\partial_{x_i}\}_{i=1,\dots,d}$ on an open neighbourhood Ω of q and an orthonormal trivializing frame $\{\nu_\alpha\}_{\alpha=1,\dots,k}$ of $N\Omega$. We define the Christoffel symbols $\Gamma_{i\alpha}^\gamma \nu_\gamma$ of the normal connection by $\Gamma_{i\alpha}^\gamma$ by $\nabla_{\partial_{x_i}}^\perp \nu_\alpha = \sum_{\gamma=1}^k \Gamma_{i\alpha}^\gamma \nu_\gamma$.

For $\nu = n^\alpha \nu_\alpha$ the vertical derivative in local coordinates is given by

$$\nabla_{\nu_\alpha}^{\text{v}} \psi(q, \nu) = \partial_{n_\alpha} \psi(x, n). \quad (50)$$

and the horizontal connection is given by

$$\nabla_{\partial_{x_i}}^{\text{h}} \psi(q, \nu) = \partial_{x_i} \psi(x, n) - \Gamma_{i\alpha}^\gamma n^\alpha \partial_{n^\gamma} \psi(x, n). \quad (51)$$

The former directly follows from the definition of ∇^{v} (Definition 1). To obtain the latter equation we note first that for a normal vector field $v = n^\alpha \nu_\alpha$ over \mathcal{C} it holds

$$(\nabla_{\partial_{x_i}}^\perp v)^\gamma = \partial_{x_i} n^\gamma + \Gamma_{i\alpha}^\gamma n^\alpha. \quad (52)$$

Now let $(w, v) \in C^1([-1, 1], N\mathcal{C})$ with

$$w(0) = q, \dot{w}(0) = \tau(q), \quad \& \quad v(0) = \nu, \nabla_{\dot{w}}^\perp v = 0.$$

Then by definition of ∇^h we have

$$\begin{aligned} \nabla_{\partial_{x_i}}^h \psi(q, \nu) &= \left. \frac{d}{ds} \right|_{s=0} \psi(w(s), v(s)) \\ &= \left. \frac{d}{ds} \right|_{s=0} \psi(w(s), \nu) + \left. \frac{d}{ds} \right|_{s=0} \psi(q, v(s)) \\ &= \partial_{x_i} \psi(q, n) + (\partial_{x_i} n^\gamma) \partial_{n^\gamma} \psi(x, n) \\ &= \partial_{x_i} \psi(q, n) - \Gamma_{i\alpha}^\gamma n^\alpha \partial_{n^\gamma} \psi(x, n) \end{aligned}$$

where we used (52) and the choice of the curve v in the last step.

Let $\tau \in \Gamma(T\mathcal{C})$ and $\psi_1, \psi_2 \in L^2(N\mathcal{C}, \bar{g}) \cap \mathcal{D}(\nabla_\tau^h)$. We now verify that ∇^h is metric, i.e. $(d\langle \psi_1 | \psi_2 \rangle_{\mathcal{H}_f})(\tau) = \langle \nabla_\tau^h \psi_1 | \psi_2 \rangle_{\mathcal{H}_f} + \langle \psi_1 | \nabla_\tau^h \psi_2 \rangle_{\mathcal{H}_f}$. Because of $\Gamma_{i\alpha}^\alpha = 0$ for all α integration by parts yields

$$\langle \Gamma_{i\alpha}^\gamma n^\alpha \partial_{n^\gamma} \psi_1 | \psi_2 \rangle_{\mathcal{H}_f} + \langle \psi_1 | \Gamma_{i\alpha}^\gamma n^\alpha \partial_{n^\gamma} \psi_2 \rangle_{\mathcal{H}_f} = 0. \quad (53)$$

Therefore we have

$$\begin{aligned} (d\langle \psi_1 | \psi_2 \rangle)(\tau) &= \tau^i \langle \partial_{x_i} \psi_1 | \psi_2 \rangle + \tau^i \langle \psi_1 | \partial_{x_i} \psi_2 \rangle \\ &= \tau^i \langle (\partial_{x_i} - \Gamma_{i\alpha}^\gamma n^\alpha \partial_{n^\gamma}) \psi_1 | \psi_2 \rangle + \tau^i \langle \psi_1 | (\partial_{x_i} - \Gamma_{i\alpha}^\gamma n^\alpha \partial_{n^\gamma}) \psi_2 \rangle \\ &= \langle \nabla_\tau^h \psi_1 | \psi_2 \rangle + \langle \psi_1 | \nabla_\tau^h \psi_2 \rangle. \end{aligned}$$

To compute the curvature we notice that the calculation from the proof of Proposition 1 in this case yields

$$R^h(\tau_1, \tau_2)\psi = \tau_1^i \tau_2^j \left((\partial_{x_i} \Gamma_{j\alpha}^\gamma - \partial_{x_j} \Gamma_{i\alpha}^\gamma) n^\alpha \partial_{n^\gamma} \psi + [\Gamma_{i\alpha}^\delta n^\alpha \partial_{n^\delta}, \Gamma_{j\beta}^\gamma n^\beta \partial_{n^\gamma}] \psi \right).$$

Using the commutator identity

$$[\Gamma_{i\alpha}^\delta n^\alpha \partial_{n^\delta}, \Gamma_{j\beta}^\gamma n^\beta \partial_{n^\gamma}] \psi = (\Gamma_{i\alpha}^\beta \Gamma_{j\beta}^\gamma - \Gamma_{j\alpha}^\beta \Gamma_{i\beta}^\gamma) n^\alpha \partial_{n^\gamma} \psi$$

we obtain that

$$\begin{aligned} R^h(\tau_1, \tau_2)\psi &= \tau_1^i \tau_2^j (\partial_{x_i} \Gamma_{j\alpha}^\gamma - \partial_{x_j} \Gamma_{i\alpha}^\gamma + \Gamma_{i\alpha}^\beta \Gamma_{j\beta}^\gamma - \Gamma_{j\alpha}^\beta \Gamma_{i\beta}^\gamma) n^\alpha \partial_{n^\gamma} \psi \\ &= \tau_1^i \tau_2^j R_{\alpha ij}^\gamma n^\alpha \partial_{n^\gamma} \psi \\ &= \bar{g}(\nu, R^\perp(\tau_1, \tau_2) \nabla^\nu \psi), \end{aligned}$$

which was the claim. \square

4 The whole story

4.1 Elliptic estimates for the Sasaki metric

Since \mathcal{C} is of bounded geometry, it has a countable covering $\{\Omega_j\}$ by contractible geodesic balls of finite multiplicity, i.e. there is $l \in \mathbb{N}$ such that each Ω_j overlaps with not more than l of the others. Furthermore there is a corresponding partition of unity $\{\xi_j \in C_0^\infty(\Omega_j)\}$ which has uniformly bounded derivatives (see [32]). We notice that $NC|_{\Omega_j}$ is trivialisable for all $j \in \mathbb{N}$ because Ω_j is contractible. Let $(x_j^i)_{i=1,\dots,d}$ be geodesic coordinates on $\Omega_j \subset \mathcal{C}$ and $(n_j^\alpha)_{\alpha=1,\dots,k}$ be bundle coordinates with respect to an orthonormal trivializing frame $\{\nu_\alpha^j\}_\alpha$ over Ω_j . We recall the coordinate formulas for ∇^v and ∇^h obtained in the proof of Lemma 7:

$$\nabla_{\partial_{\nu_\alpha}}^v \psi(q, \nu) = \partial_{n^\alpha} \psi(x, n). \quad (54)$$

and

$$\nabla_{\partial_{x^i}}^h \psi(q, \nu) = \partial_{x^i} \psi(x, n) - \Gamma_{i\alpha}^\gamma n^\alpha \partial_{n^\gamma} \psi(x, n). \quad (55)$$

In bundle coordinates the Sasaki metric has a simple form. Here we keep the convention that it is summed over repeated indices and write a^{ij} for the inverse of a_{ij} .

Proposition 2 *Let g^S be the Sasaki metric on NC defined in (9). Choose $\Omega \subset \mathcal{C}$ where the normal bundle NC is trivialisable and an orthonormal frame $\{\nu_\alpha\}_\alpha$ of $NC|_\Omega$. Define $\Gamma_{i\alpha}^\gamma$ by $\nabla_{\partial_{x^i}}^\perp \nu_\alpha = \Gamma_{i\alpha}^\gamma \nu_\gamma$. In the corresponding bundle coordinates the dual metric tensor $g_S \in \mathcal{T}_0^2(TNC)$ for all $q \in \Omega$ is given by:*

$$g_S = \begin{pmatrix} 1 & 0 \\ C^T & 1 \end{pmatrix} \begin{pmatrix} A & 0 \\ 0 & B \end{pmatrix} \begin{pmatrix} 1 & C \\ 0 & 1 \end{pmatrix},$$

where for $i, j = 1, \dots, d$ and $\alpha, \gamma, \delta = 1, \dots, k$

$$\begin{aligned} A^{ij}(q, n) &= g^{ij}(q), & B^{\gamma\delta}(q, n) &= \delta^{\gamma\delta}, \\ C_i^\gamma(q, n) &= -n^\alpha \Gamma_{i\alpha}^\gamma(q). \end{aligned}$$

In particular, $(\det(g_S)_{ab})(q, n) = (\det g_{ij})(q)$ for $a, b = 1, \dots, d + k$.

The proof was carried out by Wittich in [36]. From this expression we deduce the form of the associated Laplacian.

Corollary 3 *The Laplace-Beltrami operator associated to g_S is*

$$\Delta_S = \Delta_h + \Delta_v.$$

PROOF OF COROLLARY 3:

We set $\mu := \det g_{ij}$ and $\mu_S := \det(g_S)_{ab}$. Since $(\nu_\alpha)_{\alpha=1}^k$ is an orthonormal frame, we have that $g_{(q,0)}(\partial_{n_\alpha}, \partial_{n_\beta}) = \delta^{\alpha\beta}$. So (54) and (55) imply that

$$\Delta_v = \partial_{n^\alpha} \delta^{\alpha\beta} \partial_{n^\beta} \ \& \ \Delta_h = \mu^{-1} (\partial_{x^i} - \Gamma_{i\alpha}^\gamma n^\alpha \partial_{n^\gamma}) \mu g^{ij} (\partial_{x^j} - \Gamma_{i\alpha}^\gamma n^\alpha \partial_{n^\gamma}). \quad (56)$$

Now plugging the expression for g_S^{ab} and $\det g_S^{ab}$ from Proposition 2 into the general formula $\Delta_S = \sum_{a,b=1}^{d+k} (\mu_S)^{-1} \partial_a \mu_S g_S^{ab} \partial_b$ yields the claim. \square

Next we gather some useful properties of Δ_v , Δ_h , and ∇^h .

Lemma 8 *Let $f \in C^2(\mathbb{R})$ and $\tau \in \Gamma(T\mathcal{C})$ be arbitrary. Fix $\lambda \in \mathbb{R}$. On \mathcal{H} the following operator equations hold true:*

- i) $D_\varepsilon \Delta_v D_\varepsilon^* = \varepsilon^2 \Delta_v$, $D_\varepsilon \Delta_h D_\varepsilon^* = \Delta_h$, $D_\varepsilon V_\varepsilon D_\varepsilon^* = V_\varepsilon$,
- ii) $[\nabla_\tau^h, \Delta_v] = 0$, $[\Delta_h, \Delta_v] = 0$, $[\nabla_\tau^h, f(\langle \lambda \nu \rangle)] = 0$,
- iii) $[\Delta_v, f(\langle \lambda \nu \rangle)] = \lambda f'(\langle \lambda \nu \rangle) \left(\lambda \frac{k \langle \lambda \nu \rangle^2 - |\lambda \nu|^2}{\langle \lambda \nu \rangle^3} - \frac{2}{\langle \lambda \nu \rangle} \nabla_{\lambda \nu}^v \right) - \lambda^2 f''(\langle \lambda \nu \rangle) \frac{|\lambda \nu|^2}{\langle \lambda \nu \rangle^2}$.

We recall that $A \prec B$ means that A is operator-bounded by B with a constant independent of ε . We will have to estimate multiple applications of ∇^v and ∇^h by powers of H_ε . Central to our analysis, especially to the proof of Proposition 4 below, are the following statements:

Lemma 9 *Fix $\lambda > 0$ and $l \in \{0, 1, 2\}$. For all $m \in \mathbb{N}_0$ and $m_1 + m_2 \leq 2m$ the following operator estimates hold true:*

- i) $H_\varepsilon^m \prec (-\varepsilon^2 \Delta_h - \Delta_v + V_\varepsilon)^m \prec H_\varepsilon^m$,
- ii) $(-\Delta_v)^m (-\varepsilon^2 \Delta_h)^l \prec H_\varepsilon^{l+m}$,
- iii) $\langle \lambda \nu \rangle^m [H_\varepsilon^{l+1}, \langle \lambda \nu \rangle^{-m}] \prec H_\varepsilon^{l+1}$,
- iv) $\langle \nu \rangle^{-4m_1 - 5m_2} (\nabla^v)^{m_1} (\varepsilon \nabla^h)^{m_2} \prec H_\varepsilon^m$.

The last three estimates rely on the following estimates in bundle coordinates.

Lemma 10 *Let α, β, γ be multi-indices with $|\alpha| \leq 2l$, $|\alpha| + |\beta| \leq 2m$ and $|\gamma| = 2$. Then for all $\psi \in \mathcal{D}(H_\varepsilon^m)$*

- i) $\left(\sum_j \int_{\Omega_j} \int_{\mathbb{R}^k} |\partial_n^\alpha \psi|^2 dn \mu(x) dx \right)^{1/2} \lesssim \|(-\Delta_v)^l \psi\| + \|\psi\|$,
- ii) $\left(\sum_j \int_{\Omega_j} \int_{\mathbb{R}^k} |\partial_n^\gamma \psi|^2 dn \mu(x) dx \right)^{1/2} \lesssim \|(-\varepsilon^2 \Delta_h - \Delta_v) \psi\| + \|\psi\|$,

$$\begin{aligned}
iii) \quad & \left(\sum_j \int_{\Omega_j} \int_{\mathbb{R}^k} \langle \nu / \varepsilon \rangle^{-8(|\alpha|+|\beta|)} |\varepsilon^{|\alpha|} \partial_N^\alpha (\varepsilon^{|\beta|} \partial_x^\beta) \psi|^2 dn \mu(x) dx \right)^{1/2} \\
& \lesssim \| (-\varepsilon^2 \Delta_h - \varepsilon^2 \Delta_v + V^\varepsilon)^m \psi \| + \|\psi\|, \\
iv) \quad & \left(\sum_j \int_{\Omega_j} \int_{\mathbb{R}^k} \langle \nu \rangle^{-8(|\alpha|+|\beta|)} |\partial_n^\alpha (\varepsilon^{|\beta|} \partial_x^\beta) \psi|^2 dn \mu(x) dx \right)^{1/2} \\
& \lesssim \| (-\varepsilon^2 \Delta_h - \Delta_v + V_\varepsilon)^m \psi \| + \|\psi\|.
\end{aligned}$$

We now provide the proofs of these three technical lemmas.

PROOF OF LEMMA 8:

We fix one of the contractable balls $\Omega_j \subset \mathcal{C}$. Let $(\nu_\alpha)_{\alpha=1,\dots,k}$ be an orthonormal trivializing frame of $N\Omega_j$ and $(x_i)_{i=1,\dots,d}$ be geodesic coordinates Ω_j . Observing that $D_\varepsilon \psi(x, n) = \varepsilon^{-k/2} \psi(x, n/\varepsilon)$ and $D_\varepsilon^* \psi(x, n) = \varepsilon^{k/2} \psi(x, \varepsilon n)$ we immediately obtain i) due to (56).

Since ∇^\perp is metric, (55) implies

$$\nabla_{\partial_{x^i}}^h \psi(q, \nu) = \partial_{x^i} \psi(x, n) - \frac{1}{2} \Gamma_{i\alpha}^\gamma (n^\alpha \partial_{n^\gamma} - n^\gamma \partial_{n^\alpha}) \psi(x, n).$$

Using that $\Delta_v = \delta^{\alpha\beta} \partial_{n^\alpha} \partial_{n^\beta}$ by (56) we obtain that for any $\tau = \tau^i \partial_{x^i}$

$$[\nabla_\tau^h, \Delta_v] = \tau^i \Gamma_i^{\gamma\alpha} (\partial_{n^\alpha} \partial_{n^\gamma} - \partial_{n^\gamma} \partial_{n^\alpha}) = 0.$$

Since $(\nu_\alpha)_{\alpha=1}^k$ is an orthonormal frame, we have that $g_{(q,0)}(\partial_{n^\alpha}, \partial_{n^\beta}) = \delta^{\alpha\beta}$. This entails that $\langle \nu \rangle = \sqrt{1 + \delta_{\alpha\beta} n^\alpha n^\beta}$. Now the remaining statements follow by direct computation. \square

PROOF OF LEMMA 9:

Since D_ε and M_ρ are unitary, i) of Lemma 8 yields that i) is equivalent to

$$(H^\varepsilon)^m \prec M_\rho (-\varepsilon^2 \Delta_h - \varepsilon^2 \Delta_v + V^\varepsilon)^m M_\rho^* \prec (H^\varepsilon)^m \quad (57)$$

for all $m \in \mathbb{N}$. By choice of \bar{g} it coincides with the Sasaki metric g_S outside of $\mathcal{B}_{\delta/2}$ and, hence, so do Δ_{NC} and Δ_S . In addition, this means $\rho \equiv 1$ outside of $\mathcal{B}_{\delta/2}$ and so M_ρ is multiplication by 1 there. Then Corollary 3 implies $H^\varepsilon = M_\rho (-\varepsilon^2 \Delta_h - \varepsilon^2 \Delta_v + V^\varepsilon) M_\rho^*$ on $NC \setminus \mathcal{B}_{\delta/2}$. Hence, it suffices to prove (57) for functions with support in $\mathcal{B}_{3\delta/4} \cap \Omega_j$ by introducing suitable cutoff functions. But $\mathcal{B}_{3\delta/4} \cap \Omega_j$ is compact with respect to both \bar{g} and g^S and here both $(H^\varepsilon)^m$ and $M_\rho (-\varepsilon^2 \Delta_h - \varepsilon^2 \Delta_v + V^\varepsilon)^m M_\rho^*$ are elliptic operators with bounded coefficients of order $2m$. Thus (57) follows from the usual elliptic estimates which are uniform in j because $\mathcal{B}_{3\delta/4}$ is of bounded geometry with respect to both \bar{g} and g^S .

We recall that $V_\varepsilon \in C_b^\infty(\mathcal{C}, C_b^\infty(N_q\mathcal{C}))$ and turn to ii). By i) we may replace H_ε by $-\varepsilon^2\Delta_h - \Delta_v + V_\varepsilon$. We first prove the statement for $l = 0$ inductively. In view of (56) Lemma 10 implies that $-\Delta_v \prec -\varepsilon^2\Delta_h - \Delta_v$ and thus also $-\varepsilon^2\Delta_h \prec -\varepsilon^2\Delta_h - \Delta_v$. So due to the boundedness of V_ε the triangle inequality yields the statement for $m = 1$ and

$$-\varepsilon^2\Delta_h \prec -\varepsilon^2\Delta_h - \Delta_v + V_\varepsilon. \quad (58)$$

In the following we will write $A \prec B \dot{+} C$, if $\|A\psi\| \lesssim \|B\psi\| + \|C\psi\| + \|\psi\|$. We note that with this notation $A \prec B$ implies $AC \prec BC \dot{+} C$.

Now we assume that the statement is true for some $m \in \mathbb{N}_0$. By the spectral calculus lower powers of $(-\varepsilon^2\Delta_h - \Delta_v + V_\varepsilon)$ are operator-bounded by higher powers. In addition, Δ_v and Δ_h commute by Lemma 8. Then we obtain the statement for $m + 1$ via

$$\begin{aligned} (-\Delta_v)^{m+1} &\prec (-\varepsilon^2\Delta_h - \Delta_v + V_\varepsilon)(-\Delta_v)^m \dot{+} (-\Delta_v)^m \\ &= (-\Delta_v)^m(-\varepsilon^2\Delta_h - \Delta_v + V_\varepsilon) + [V_\varepsilon, (-\Delta_v)^m] \dot{+} (-\Delta_v)^m \\ &\prec (-\varepsilon^2\Delta_h - \Delta_v + V_\varepsilon)^{m+1} \dot{+} (-\Delta_v)^m \\ &\prec (-\varepsilon^2\Delta_h - \Delta_v + V_\varepsilon)^{m+1}. \end{aligned}$$

Here we used $V_\varepsilon \in C_b^\infty(\mathcal{C}, C_b^\infty(N_q\mathcal{C}))$, $\Delta_v = \delta^{\alpha\beta}\partial_{n^\alpha}\partial_{n^\beta}$ locally, and i) of Lemma 10 to bound $[V_\varepsilon, (-\Delta_v)^m]$ by $(-\Delta_v)^m$. Using $[\Delta_v, \Delta_h] = 0$ and (58) we have

$$\begin{aligned} (-\Delta_v)^m(-\varepsilon^2\Delta_h) &= (-\varepsilon^2\Delta_h)(-\Delta_v)^m \\ &\prec (-\varepsilon^2\Delta_h - \Delta_v + V)(-\Delta_v)^m \dot{+} (-\Delta_v)^m. \end{aligned}$$

Continuing as before we obtain the claim for $l = 1$. Furthermore

$$\begin{aligned} (-\Delta_v)^m(-\varepsilon^2\Delta_h)^2 &= (-\varepsilon^2\Delta_h)(-\Delta_v)^m(-\varepsilon^2\Delta_h) \\ &\prec (-\varepsilon^2\Delta_h - \Delta_v + V_\varepsilon)(-\Delta_v)^m(-\varepsilon^2\Delta_h) \\ &\quad \dot{+} (-\Delta_v)^m(-\varepsilon^2\Delta_h) \\ &= (-\Delta_v)^m(-\varepsilon^2\Delta_h)(-\varepsilon^2\Delta_h - \Delta_v + V_\varepsilon) \\ &\quad + [V_\varepsilon, (-\Delta_v)^m(-\varepsilon^2\Delta_h)] \dot{+} (-\varepsilon^2\Delta_h - \Delta_v + V_\varepsilon)^{m+1} \\ &\prec (-\varepsilon^2\Delta_h - \Delta_v + V_\varepsilon)^{m+2} \dot{+} [V_\varepsilon, (-\Delta_v)^m(-\varepsilon^2\Delta_h)]. \end{aligned}$$

To handle the last term we notice that

$$\Delta_h = \sum_{i=1}^d \nabla_{\tau_i}^h \nabla_{\tau_i}^h \quad (59)$$

for orthonormal sections $(\tau_i)_{i=1,\dots,d}$ of $T\Omega_j$. Then

$$\begin{aligned}
[V_\varepsilon, (-\Delta_v)^m (-\varepsilon^2 \Delta_h)] &= [V_\varepsilon, (-\Delta_v)^m] (-\varepsilon^2 \Delta_h) + (-\Delta_v)^m [V_\varepsilon, (-\varepsilon^2 \Delta_h)] \\
&\prec (-\Delta_v)^m (-\varepsilon^2 \Delta_h) \dot{+} (-\Delta_v)^m \sum_{j=1}^d \varepsilon \nabla_{\tau_j}^h \dot{+} (-\Delta_v)^m \\
&= \sum_{j=1}^d \varepsilon \nabla_{\tau_j}^h (-\Delta_v)^m \dot{+} (-\varepsilon^2 \Delta_h) (-\Delta_v)^m \dot{+} (-\Delta_v)^m \\
&\prec (-\varepsilon^2 \Delta_h) (-\Delta_v)^m \dot{+} (-\Delta_v)^m \\
&\prec (-\varepsilon^2 \Delta_h - \Delta_v + V_\varepsilon)^{m+2}
\end{aligned}$$

because

$$\begin{aligned}
\int_{NC} \delta^{ij} \varepsilon \nabla_{\tau_i}^h \psi^* \varepsilon \nabla_{\tau_j}^h \psi d\mu \otimes d\nu &= \int_{NC} g(\varepsilon \nabla^h \psi^*, \varepsilon \nabla^h \psi) d\mu \otimes d\nu \\
&= \langle \psi | -\varepsilon^2 \Delta_h \psi \rangle \\
&\leq \| -\varepsilon^2 \Delta_h \psi \| + \|\psi\|.
\end{aligned}$$

We prove iii) only for $l = 2$ which is the hardest case. We notice that

$$\begin{aligned}
\langle \lambda\nu \rangle^m [H_\varepsilon^3, \langle \lambda\nu \rangle^{-m}] &= \langle \lambda\nu \rangle^m [H_\varepsilon, \langle \lambda\nu \rangle^{-m}] H_\varepsilon^2 + \langle \lambda\nu \rangle^m H_\varepsilon [H_\varepsilon, \langle \lambda\nu \rangle^{-m}] H_\varepsilon \\
&\quad + \langle \lambda\nu \rangle^m H_\varepsilon^2 [H_\varepsilon, \langle \lambda\nu \rangle^{-m}].
\end{aligned}$$

We also only treat the hardest of these summands which is the last one. Inside of $\mathcal{B}_{3\delta/4}$ the estimate iv) can be reduced to standard elliptic estimates as in ii). Therefore we may again replace H_ε by $-\varepsilon^2 \Delta_h - \Delta_v + V_\varepsilon$. In view of ii) of Lemma 8 we have

$$\begin{aligned}
&\langle \lambda\nu \rangle^m (-\varepsilon^2 \Delta_h - \Delta_v + V_\varepsilon)^2 [-\varepsilon^2 \Delta_h - \Delta_v + V_\varepsilon, \langle \lambda\nu \rangle^{-m}] \\
&= \langle \lambda\nu \rangle^m (-\varepsilon^2 \Delta_h - \Delta_v + V_\varepsilon)^2 [-\Delta_v, \langle \lambda\nu \rangle^{-m}] \\
&= \langle \lambda\nu \rangle^m (-\Delta_v + V_\varepsilon)^2 [-\Delta_v, \langle \lambda\nu \rangle^{-m}] + \langle \lambda\nu \rangle^m [-\Delta_v, \langle \lambda\nu \rangle^{-m}] (-\varepsilon^2 \Delta_h)^2 \\
&\quad + 2 \langle \lambda\nu \rangle^m (-\Delta_v + V_\varepsilon) [-\Delta_v, \langle \lambda\nu \rangle^{-m}] (-\varepsilon^2 \Delta_h) \\
&\quad + \langle \lambda\nu \rangle^m [-\varepsilon^2 \Delta_h, V_\varepsilon] [-\Delta_v, \langle \lambda\nu \rangle^{-m}]
\end{aligned}$$

We note that because of $\Delta_v = \delta^{\alpha\beta} \partial_{n_\alpha} \partial_{n_\beta}$ and iii) of Lemma 8 the differential operator $\langle \lambda\nu \rangle^m (-\Delta_v + V_\varepsilon)^l [-\Delta_v, \langle \lambda\nu \rangle^{-m}]$ contains only normal partial derivatives and has bounded coefficients for any l . So by i) of Lemma 10 it is bounded by $(-\Delta_v)^{l+1}$. Then ii) of this Lemma immediately allows to bound the first three terms by $(-\varepsilon^2 \Delta_h - \Delta_v + V_\varepsilon)^3$. The last term can be treated

as follows:

$$\begin{aligned}
\langle \lambda\nu \rangle^m [-\varepsilon^2 \Delta_h, V_\varepsilon] [-\Delta_v, \langle \lambda\nu \rangle^{-m}] &= [-\varepsilon^2 \Delta_h, V_\varepsilon] \langle \lambda\nu \rangle^m [-\Delta_v, \langle \lambda\nu \rangle^{-m}] \\
&\prec -\varepsilon^2 \Delta_h \langle \lambda\nu \rangle^m [-\Delta_v, \langle \lambda\nu \rangle^{-m}] \\
&\quad \dagger \langle \lambda\nu \rangle^m [-\Delta_v, \langle \lambda\nu \rangle^{-m}] \\
&= \langle \lambda\nu \rangle^m [-\Delta_v, \langle \lambda\nu \rangle^{-m}] (-\varepsilon^2 \Delta_h) \\
&\quad \dagger \langle \lambda\nu \rangle^m [-\Delta_v, \langle \lambda\nu \rangle^{-m}] \\
&\prec (-\Delta_v) (-\varepsilon^2 \Delta_h) \dagger (-\varepsilon^2 \Delta_h) \dagger (-\Delta_v)
\end{aligned}$$

which is bounded by $(-\varepsilon^2 \Delta_h - \Delta_v + V_\varepsilon)^2$ again due to ii).

In view of (54) and (55) the estimate iv) follows directly from iv) of Lemma 10 and i) of this Lemma. A polynomial weight is necessary because here the unbounded geometry of $(N\mathcal{C}, \bar{g})$ really comes into play. In i) we could avoid this using that the operators differ only on a set of bounded geometry, while in ii) and iii) the number of horizontal derivatives was small! \square

PROOF OF LEMMA 10:

The first estimate is just an elliptic estimate on each fibre and thus a consequence of the usual elliptic estimates on \mathbb{R}^k . To see this we note that $\Delta_v = \delta^{\alpha\beta} \partial_{n_\alpha} \partial_{n_\beta}$ is the Laplace operator on the fibers (see the proof of Corollary 3) and that the measure $d\mu \otimes d\nu = dn \mu(x) dx$ is independent of n .

Concerning ii) and iii) we will derive the stated a priori estimates for smooth functions that decay fast enough. Then it is only a matter of standard density and approximation arguments to obtain the estimates for all $\psi \in \mathcal{D}(H_\varepsilon^m)$.

To deduce the second estimate we aim to show that

$$\begin{aligned}
&\sum_{|\gamma|=2} \int_{\Omega_j} \int_{\mathbb{R}^k} |\partial_n^\gamma \Psi|^2 dn \mu(x) dx \\
&\lesssim \sum_{|\gamma|=2} \int_{\Omega_j} \int_{\mathbb{R}^k} |\partial_n^\gamma \Psi| (|(-\varepsilon^2 \Delta_h - \Delta_v) \Psi| + |\varepsilon \nabla^h \psi| + |\Psi|) dn \mu(x) dx. \quad (60)
\end{aligned}$$

with a constant independent of j . Then the claim follows from the Cauchy-Schwartz inequality and $\| |\varepsilon \nabla^h \psi| \| = \langle \psi | -\varepsilon^2 \Delta_h \psi \rangle^{\frac{1}{2}} \leq \langle \psi | (-\varepsilon^2 \Delta_h - \Delta_v) \psi \rangle^{\frac{1}{2}}$ which is smaller than $\|(-\varepsilon^2 \Delta_h - \Delta_v) \Psi\| + \|\Psi\|$.

On the one hand there are $\alpha, \beta \in \{1, \dots, k\}$ such that

$$\begin{aligned}
\int_{\Omega_j} \int_{\mathbb{R}^k} |\partial_n^\gamma \Psi|^2 dn \mu(x) dx &= \int_{\Omega_j} \int_{\mathbb{R}^k} \partial_{n^\alpha} \partial_{n^\beta} \psi^* \partial_{n^\alpha} \partial_{n^\beta} \psi dn \mu(x) dx \\
&= \int_{\Omega_j} \int_{\mathbb{R}^k} \partial_{n^\beta} \partial_{n^\beta} \psi^* \partial_{n^\alpha} \partial_{n^\alpha} \psi dn \mu(x) dx \\
&= \int_{\Omega_j} \int_{\mathbb{R}^k} \partial_{n^\beta} \partial_{n^\beta} \psi^* \Delta_v \psi dn \mu(x) dx.
\end{aligned}$$

On the other hand

$$\begin{aligned}
0 &\leq \int_{\Omega_j} \int_{\mathbb{R}^k} g(\varepsilon \nabla^h \partial_{n^\beta} \psi^*, \varepsilon \nabla^h \partial_{n^\beta} \psi) \, dn \, \mu(x) dx \\
&= \int_{\Omega_j} \int_{\mathbb{R}^k} g^{il} \varepsilon (\partial_{x^i} + \Gamma_{i\zeta}^\alpha n^\zeta \partial_{n^\alpha}) \partial_{n^\beta} \psi^* \varepsilon (\partial_{x^l} + \Gamma_{l\delta}^\eta n^\delta \partial_{n^\eta}) \partial_{n^\beta} \psi \, dn \, \mu(x) dx \\
&= \int_{\Omega_j} \int_{\mathbb{R}^k} -g^{il} \varepsilon (\partial_{x^i} + \Gamma_{i\zeta}^\alpha n^\zeta \partial_{n^\alpha}) \partial_{n^\beta} \partial_{n^\beta} \psi^* \varepsilon (\partial_{x^l} + \Gamma_{l\delta}^\eta n^\delta \partial_{n^\eta}) \psi \\
&\quad - \varepsilon g^{il} \varepsilon (\partial_{x^i} + \Gamma_{i\zeta}^\alpha n^\zeta \partial_{n^\alpha}) \partial_{n^\beta} \psi^* \Gamma_{l\beta}^\eta \partial_{n^\eta} \psi \\
&\quad - \varepsilon g^{il} \Gamma_{i\beta}^\alpha \partial_{n^\alpha} \partial_{n^\beta} \psi^* \varepsilon (\partial_{x^l} + \Gamma_{l\delta}^\eta n^\delta \partial_{n^\eta}) \psi \, dn \, \mu(x) dx \\
&= \int_{\Omega_j} \int_{\mathbb{R}^k} \partial_{n^\beta} \partial_{n^\beta} \psi^* \varepsilon^2 \Delta_h \psi + \varepsilon^2 g^{ij} \Gamma_{i\beta}^\alpha \partial_{n^\alpha} \psi^* \Gamma_{l\beta}^\eta \partial_{n^\eta} \psi \\
&\quad - 2\varepsilon \operatorname{Im} \left(g^{il} \Gamma_{i\beta}^\alpha \partial_{n^\alpha} \partial_{n^\beta} \psi^* \varepsilon (\partial_{x^l} + \Gamma_{l\delta}^\eta n^\delta \partial_{n^\eta}) \psi \right) \, dn \, \mu(x) dx
\end{aligned}$$

with $\operatorname{Im}(a)$ the imaginary part of a . When we add the last two calculations and sum up over all multi-indices γ with $|\gamma| = 2$, we obtain the desired $(-\varepsilon^2 \Delta_h - \Delta_v)$ -term. However, we have to take care of the two error terms in the latter estimate:

$$\begin{aligned}
&\int_{\Omega_j} \int_{\mathbb{R}^k} g^{il} \Gamma_{i\beta}^\alpha \partial_{n^\alpha} \psi^* \Gamma_{l\beta}^\eta \partial_{n^\eta} \psi \, dn \, \mu(x) dx \\
&= \int_{\Omega_j} \int_{\mathbb{R}^k} -g^{il} \Gamma_{i\beta}^\alpha \partial_{n^\eta} \partial_{n^\alpha} \psi^* \Gamma_{l\beta}^\eta \psi \, dn \, \mu(x) dx \\
&\leq \sup |g^{il} \Gamma_{i\beta}^\alpha \Gamma_{l\beta}^\eta| \sum_{|\gamma|=2} \int_{\Omega_j} \int_{\mathbb{R}^k} |\partial_{n^\eta} \partial_{n^\alpha} \psi^*| |\psi| \, dn \, \mu(x) dx
\end{aligned}$$

and

$$\begin{aligned}
&\int_{\Omega_j} \int_{\mathbb{R}^k} 2 \operatorname{Im} \left(g^{il} \Gamma_{i\beta}^\alpha \partial_{n^\alpha} \partial_{n^\beta} \psi^* \varepsilon (\partial_{x^l} + \Gamma_{l\delta}^\eta n^\delta \partial_{n^\eta}) \psi \right) \, dn \, \mu(x) dx \\
&\leq 2 \sup |(g^{il})^{\frac{1}{2}} \Gamma_{i\beta}^\alpha| \sum_{|\gamma|=2} \int_{\Omega_j} \int_{\mathbb{R}^k} |\partial_{n^\alpha} \partial_{n^\beta} \psi| |\varepsilon \nabla^h \psi| \, dn \, \mu(x) dx.
\end{aligned}$$

Since g^{il} and $\Gamma_{i\beta}^\alpha$ can be bounded independently of j due to the bounded geometry and the smooth embedding of \mathcal{C} , this yields (60).

We now turn to the third part. We notice that the powers of ε on both sides match because then all derivatives carry an ε . Therefore we may drop all the ε 's in our calculations to deduce the last estimate. Since we have stated the estimate with a non-optimal power of $\langle \nu \rangle$, there is also no need to distinguish

between normal and tangential derivatives anymore. So the multi-index α will be supposed to allow for both normal and tangential derivatives. We recall that $\Delta_S = \Delta_h + \Delta_v$. We will prove by induction that for all $m \in \mathbb{N}_0$

$$\begin{aligned} & \left(\sum_{|\alpha| \leq m+2} \int_{\Omega_j} \int_{\mathbb{R}^k} \langle \nu \rangle^{-8|\alpha|} |\partial^\alpha \psi|^2 \mu \, dn \, dx \right)^{\frac{1}{2}} \\ & \lesssim \left(\sum_{|\beta| \leq m} \int_{\Omega_j} \int_{\mathbb{R}^k} \langle \nu \rangle^{-8|\beta|} |\partial^\beta (-\Delta_S + V)\psi|^2 \mu \, dn \, dx \right)^{\frac{1}{2}} + \|\psi\| \quad (61) \end{aligned}$$

with a constant independent of j . Applying this estimate iteratively we obtain our claim because due to the spectral calculus $(-\Delta_S + V)^l$ is operator-bounded by $(-\Delta_S + V)^m$ for $l \leq m$.

Before we start with the induction we notice that g_S^{ab} is positive definit with a constant that is bounded from below by $\langle \nu \rangle^{-2}$ times a constant depending only on the geometry of \mathcal{C} . More precisely, it depends on $\inf g^{ij}$ and $\sup \Gamma_{i\gamma}^\beta$ which are both uniformly bounded due to our assumptions on \mathcal{C} and our choice of coordinates.

We now turn to the case $m = 0$. For $|\alpha| = 0$ there is nothing to prove. For $|\alpha| = 1$ we have

$$\begin{aligned} \sum_{|\alpha|=1} \int_{\Omega_j} \int_{\mathbb{R}^k} \langle \nu \rangle^{-8} |\partial^\alpha \psi|^2 \mu \, dn \, dx & \lesssim \int_{\Omega_j} \int_{\mathbb{R}^k} g_S^{ab} \partial_a \psi^* \partial_b \psi \mu \, dn \, dx \\ & = \int_{\Omega_j} \int_{\mathbb{R}^k} \psi^* ((-\Delta_S + V)\psi - V\psi) \mu \, dn \, dx \\ & \leq \|\psi\| (\|(-\Delta_S + V)\psi\| + \sup |V| \|\psi\|) \\ & \leq \|(-\Delta_S + V)\psi\|^2 + \|\psi\|^2 \\ & \leq (\|(-\Delta_S + V)\psi\| + \|\psi\|)^2. \quad (62) \end{aligned}$$

Taking the square root yields the desired estimate in this case. For $|\alpha| = 2$

we have

$$\begin{aligned}
& \sum_{|\alpha|=2} \int_{\Omega_j} \int_{\mathbb{R}^k} \langle \nu \rangle^{-16} |\partial^\alpha \psi|^2 \mu \, dn \, dx \\
& \lesssim \sum_c \int_{\Omega_j} \int_{\mathbb{R}^k} \langle \nu \rangle^{-14} g_S^{ab} \partial_a \partial_c \psi^* \partial_b \partial_c \psi \mu \, dn \, dx \\
& = \sum_c \int_{\Omega_j} \int_{\mathbb{R}^k} -\langle \nu \rangle^{-14} g_S^{ab} \partial_a \partial_c \partial_c \psi^* \partial_b \psi \\
& \quad - \mu^{-1} (\partial_c \mu \langle \nu \rangle^{-14} g_S^{ab}) \partial_a \partial_c \psi^* \partial_b \psi \mu \, dn \, dx \\
& = \sum_c \int_{\Omega_j} \int_{\mathbb{R}^k} \langle \nu \rangle^{-14} \partial_c \partial_c \psi^* (\Delta_S - V + V) \psi \\
& \quad - \left(\mu^{-1} (\partial_c \mu \langle \nu \rangle^{-14} g_S^{ab}) \partial_a \partial_c \psi^* - (\partial_a \langle \nu \rangle^{-14}) g_S^{ab} \partial_c \partial_c \psi^* \right) \partial_b \psi \mu \, dn \, dx \\
& \lesssim \sum_{|\alpha|=2} \int_{\Omega_j} \int_{\mathbb{R}^k} \langle \nu \rangle^{-8} |\partial^\alpha \psi| \left(|(-\Delta_S + V) \psi| + |V| |\psi| + \langle \nu \rangle^{-4} |\partial_b \psi| \right) \mu \, dn \, dx
\end{aligned}$$

which yields (61) via (62) when we apply the Cauchy-Schwartz inequality and divide by both sides by the square root of the left-hand side. Here we used that both $\mu^{-1} (\partial_c \mu \langle \nu \rangle^{-14} g_S^{ab})$ and $(\partial_a \langle \nu \rangle^{-14}) g_S^{ab}$ are bounded by $\langle \nu \rangle^{-12}$. This is due to the facts that g_S^{ab} and its derivatives are bounded by $\langle \nu \rangle^2$ and that any derivative of $\langle \nu \rangle^l = \sqrt{1 + \delta_{\alpha\beta} n^\alpha n^\beta}^l$ is bounded by $\langle \nu \rangle^l$. We will use these facts also in the following calculation.

We assume now that (61) is true for some fixed $m \in \mathbb{N}_0$. Then it suffices to consider multi-indices with modulus $m + 3$ to show the statement for $m + 1$.

We have

$$\begin{aligned}
& \sum_{|\alpha|=m+3} \int_{\Omega_j} \int_{\mathbb{R}^k} \langle \nu \rangle^{-8|\alpha|} |\partial^\alpha \psi|^2 \mu \, dn \, dx \\
& \lesssim \sum_{|\tilde{\alpha}|=m+2} \int_{\Omega_j} \int_{\mathbb{R}^k} \langle \nu \rangle^{-8|\tilde{\alpha}|-6} g_S^{ab} \partial_a \partial^{\tilde{\alpha}} \psi^* \partial_b \partial^{\tilde{\alpha}} \psi \mu \, dn \, dx \\
& = \sum_{|\tilde{\alpha}|=m+2} \int_{\Omega_j} \int_{\mathbb{R}^k} \langle \nu \rangle^{-8|\tilde{\alpha}|-6} \partial^{\tilde{\alpha}} \psi^* (-\Delta_S) \partial^{\tilde{\alpha}} \psi \\
& \quad - \partial^{\tilde{\alpha}} \psi^* (\partial_a \langle \nu \rangle^{-8|\tilde{\alpha}|-6}) g_S^{ab} \partial_b \partial^{\tilde{\alpha}} \psi \mu \, dn \, dx \\
& = \sum_{|\tilde{\alpha}|=m+2} \int_{\Omega_j} \int_{\mathbb{R}^k} \langle \nu \rangle^{-8|\tilde{\alpha}|-6} \partial^{\tilde{\alpha}} \psi^* \partial^{\tilde{\alpha}} (-\Delta_S) \psi \\
& \quad - \partial^\alpha \psi^* \left((\partial_a \langle \nu \rangle^{-8|\tilde{\alpha}|-6}) g_S^{ab} \partial_b \partial^{\tilde{\alpha}} \psi + \langle \nu \rangle^{-8|\alpha|-6} [\Delta_S, \partial^{\tilde{\alpha}}] \psi \right) \mu \, dn \, dx \\
& \lesssim \sum_{|\alpha|=m+3} \sum_{|\beta|=m+1} \int_{\Omega_j} \int_{\mathbb{R}^k} \langle \nu \rangle^{-4|\alpha|} |\partial^\alpha \psi| \langle \nu \rangle^{-4|\beta|} |\partial^\beta (-\Delta_S) \psi| \mu \, dn \, dx \\
& \quad + \sum_{|\alpha|=m+3} \sum_{|\tilde{\alpha}|=m+2} \int_{\Omega_j} \int_{\mathbb{R}^k} \langle \nu \rangle^{-4|\tilde{\alpha}|} |\partial^{\tilde{\alpha}} \psi| \langle \nu \rangle^{-4|\alpha|} |\partial^\alpha \psi| \mu \, dn \, dx.
\end{aligned}$$

Using again the Cauchy-Schwartz inequality and applying the induction assumption to the $\tilde{\alpha}$ -term we are almost done with the proof of (61) for $m+1$. We only have to introduce V in the Laplace term. When we put it in and use the triangle inequality we are left with the following error term:

$$\begin{aligned}
& \sum_{|\beta|=m+1} \int_{\Omega_j} \int_{\mathbb{R}^k} \langle \nu \rangle^{-8|\beta|} |\partial^\beta V \psi|^2 \mu \, dn \, dx \\
& = \sum_{|\alpha|+|\beta|=m+1} \int_{\Omega_j} \int_{\mathbb{R}^k} \langle \nu \rangle^{-8|\alpha|} |\partial^\alpha V|^2 \langle \nu \rangle^{-8|\beta|} |\partial^\beta \psi|^2 \mu \, dn \, dx.
\end{aligned}$$

In order to apply the induction assumption to this expression, we have to bound $\sup \langle \nu \rangle^{-8|\alpha|} |\partial^\alpha V|^2$. To be able to use $V \in C_b^\infty(\mathcal{C}, C_b^\infty(N_q \mathcal{C}))$ we have to replace the normal derivatives in ∂^α by ∇^v and the tangential derivatives by ∇^h . However, in view of (54) and (55) this costs at most a factor $\langle \nu \rangle^{-1}$ for each derivative.

To see that iv) is just a reformulation of iii), we put $n = N/\varepsilon$, replace ψ with $D_\varepsilon \psi$, and use that $(-\varepsilon^2 \Delta_h - \varepsilon^2 \Delta_v + V^\varepsilon) D_\varepsilon = D_\varepsilon (-\varepsilon^2 \Delta_h - \Delta_v + V_\varepsilon)$ by Lemma 8. \square

We still have to give the proof of Lemma 3 from Section 3.2. It was postponed because it makes use of Lemma 10.

PROOF OF LEMMA 3 (SECTION 3.2):

All statements in i) and ii) are easily verified by using the substitution rule. To show iii) we first verify that $(H_{\mathcal{A}}^\varepsilon A^* - A^* H^\varepsilon) \mathcal{P}^\varepsilon$ is in $\mathcal{L}(\mathcal{D}(H^\varepsilon), L^2(\mathcal{A}, d\tau))$ at all. For $A^* H^\varepsilon \mathcal{P}^\varepsilon$ this immediately follows from ii) and Corollary 2. So we have to show that $A^* \mathcal{P}^\varepsilon \in \mathcal{L}(\mathcal{D}(H^\varepsilon), \mathcal{D}(H_{\mathcal{A}}^\varepsilon))$. By Corollary 2 we have

$$\|H_{\mathcal{A}}^\varepsilon A^* \mathcal{P}^\varepsilon\|_{\mathcal{L}(\mathcal{D}(H^\varepsilon), \mathcal{D}(H_{\mathcal{A}}^\varepsilon))} \lesssim \|H_{\mathcal{A}}^\varepsilon A^* \langle \nu/\varepsilon \rangle^{-l}\|_{\mathcal{L}(\mathcal{D}(H^\varepsilon), \mathcal{D}(H_{\mathcal{A}}^\varepsilon))}$$

for any $l \in \mathbb{N}$ and ψ . Now we again fix $\Omega_j \subset \mathcal{C}$ and choose geodesic coordinates $(x_j^i)_{i=1, \dots, d}$ and bundle coordinates $(n_j^\alpha)_{\alpha=1, \dots, k}$ with respect to an orthonormal trivializing frame $\{\nu_\alpha^j\}_\alpha$ over Ω_j . When we write down A^* and $H_{\mathcal{A}}^\varepsilon$ in these coordinates, we will end up with coefficients that grow polynomially due to our choice of the diffeomorphism Φ . However, this is compensated by $\langle \nu/\varepsilon \rangle^{-l}$. Choosing l big enough allows us to apply Lemma 10 iii) to obtain a bound by $-\varepsilon^2 \Delta_{\mathfrak{h}} - \varepsilon^2 \Delta_{\mathfrak{v}} + V^\varepsilon$. In the proof of Lemma 9 ii) it was shown that $-\varepsilon^2 \Delta_{\mathfrak{h}} - \varepsilon^2 \Delta_{\mathfrak{v}} + V^\varepsilon \prec H^\varepsilon$. Hence, $A^* \mathcal{P}^\varepsilon \in \mathcal{L}(\mathcal{D}(H^\varepsilon), \mathcal{D}(H_{\mathcal{A}}^\varepsilon))$. With the same arguments one also sees that $\|\langle \nu/\varepsilon \rangle^3 (H_{\mathcal{A}}^\varepsilon A^* - A^* H^\varepsilon) \mathcal{P}^\varepsilon\|_{\mathcal{L}(\mathcal{D}(H^\varepsilon), \mathcal{H})} \lesssim 1$. Since \bar{g} is by definition the pullback of $g_{\mathcal{A}}$ on $\mathcal{B}_{\delta/2}$, the operators $H_{\mathcal{A}}^\varepsilon A^*$ and $A^* H^\varepsilon$ coincide on $\mathcal{B}_{\delta/2}$. But outside of $\mathcal{B}_{\delta/2}$, i.e. for $|\nu| \geq \delta/2$, we have that

$$\langle \nu/\varepsilon \rangle^{-3} = (\varepsilon/\sqrt{\varepsilon^2 + |\nu|^2})^3 \leq 4\varepsilon^3/\delta^3.$$

Hence, $|\chi_{\mathcal{B}_{\delta/2}}^c \langle \nu/\varepsilon \rangle^{-3}| \lesssim \varepsilon^3$ with $\chi_{\mathcal{B}_{\delta/2}}^c$ the characteristic function of $\mathcal{B}_\delta \setminus \mathcal{B}_{\delta/2}$. Therefore we may estimate

$$\begin{aligned} & \| (H_{\mathcal{A}}^\varepsilon A^* - A^* H^\varepsilon) \mathcal{P}^\varepsilon \|_{\mathcal{L}(\mathcal{D}(H^\varepsilon), \mathcal{H})} \\ &= \| \chi_{\mathcal{B}_{\delta/2}}^c (H_{\mathcal{A}}^\varepsilon A^* - A^* H^\varepsilon) \mathcal{P}^\varepsilon \|_{\mathcal{L}(\mathcal{D}(H^\varepsilon), \mathcal{H})} \\ &\lesssim |\chi_{\mathcal{B}_{\delta/2}}^c \langle \nu/\varepsilon \rangle^{-3}| \| \langle \nu/\varepsilon \rangle^3 (H_{\mathcal{A}}^\varepsilon A^* - A^* H^\varepsilon) \mathcal{P}^\varepsilon \|_{\mathcal{L}(\mathcal{D}(H^\varepsilon), \mathcal{H})} \\ &\lesssim \varepsilon^3 \| \langle \nu/\varepsilon \rangle^3 (H_{\mathcal{A}}^\varepsilon A^* - A^* H^\varepsilon) \mathcal{P}^\varepsilon \|_{\mathcal{L}(\mathcal{D}(H^\varepsilon), \mathcal{H})} \\ &\lesssim \varepsilon^3 \end{aligned}$$

which was the claim. \square

4.2 Expansion of the Hamiltonian

In order to expand the Hamiltonian H_ε in powers of ε it is crucial to expand the metric \bar{g} around \mathcal{C} because it is part of the Laplace-Beltrami operator. The use of the expansion will be justified by the fast decay of functions from the relevant subspaces P_0 and P_ε .

We introduce Fermi coordinates by choosing a fixed reference frame and provide an explicit expression for expansion of the inverse metric tensor with respect to these coordinates.

Proposition 3 *Let (\mathcal{A}, \bar{g}) be a Riemannian manifold and (\mathcal{C}, g) an isometrically embedded submanifold. Choose $\Omega \subset \mathcal{C}$ where the normal bundle NC is trivializable and an orthonormal frame $\{\nu_\alpha\}_\alpha$ of $NC|_\Omega$. In the corresponding bundle coordinates the inverse metric tensor $\bar{g} \in \mathcal{T}_2^0(\mathcal{A})$ has the following expansion for all $q \in \Omega$:*

$$\bar{g} = \begin{pmatrix} 1 & 0 \\ C^T & 1 \end{pmatrix} \begin{pmatrix} A & 0 \\ 0 & B \end{pmatrix} \begin{pmatrix} 1 & C \\ 0 & 1 \end{pmatrix} + r_1,$$

where for $i, j, l, m = 1, \dots, d$ and $\alpha, \beta, \gamma, \delta = 1, \dots, k$

$$\begin{aligned} A^{ij}(q, n) &= g^{ij}(q) + n^\alpha (W_{\alpha l}^i g^{lj} + g^{il} W_{\alpha j}^l)(q) \\ &\quad + n^\alpha n^\beta (3 W_{\alpha m}^i g^{ml} W_{\beta l}^j + R_{\alpha \beta}^i{}^j)(q), \\ B^{\gamma\delta}(q, n) &= \delta_{\gamma\delta} + \frac{1}{3} n^\alpha n^\beta R_{\alpha \beta}^{\gamma \delta}(q), \\ C_i^\gamma(q, n) &= -n^\alpha \Gamma_{i\alpha}^\gamma(q) + \frac{2}{3} n^\alpha n^\beta R_{\alpha i \beta}^\gamma(q). \end{aligned}$$

Here R denotes the curvature tensor of \mathcal{A} and W_α is the Weingarten mapping corresponding to ν_α , i.e. $\mathcal{W}(\nu_\alpha)$ (see the appendix for definitions and conventions). The remainder term r_1 and its derivatives are bounded by $|n|^3$.

For the proof we refer to the recent work of Wittich [36]. Wittich does not calculate the second correction to C but it is easily deducible from his proof. Furthermore r_1 is only locally bounded by $|n|^3$ in [36]. To see that the global bound is true for \bar{g} we recall that outside of $\mathcal{B}_{\delta/2}$ it coincides with g_S , which was explicitly given in Proposition 2. Comparing the expressions for \bar{g} and g_S we obtain a bound by $|n|^2$ which is bounded by $|n|^3$ for $|n| \geq \delta/2$. In addition, we need to know the expansion of the extra potential occurring in Lemma 1, which is also provided in [36]:

Lemma 11 *For $\rho := d\bar{\mu}/d\sigma$ with $d\sigma = d\mu \otimes d\nu$ it holds*

$$V_\rho = -\frac{1}{4} \bar{g}(\eta, \eta) + \frac{1}{2} \kappa - \frac{1}{6} (\bar{\kappa} + \text{tr}_C \bar{\text{Ric}} + \text{tr}_C \bar{\text{R}}) + r_2 =: V_{\text{geom}} + r_2,$$

where η is the mean curvature normal, $\kappa, \bar{\kappa}$ are the scalar curvatures of \mathcal{C} and \mathcal{A} , $\text{tr}_C \bar{\text{Ric}}, \text{tr}_C \bar{\text{R}}$ are the partial traces with respect to \mathcal{C} of the Ricci and the Riemann tensor of \mathcal{A} and r_2 is bounded by $|n|$.

With these two inputs the proof of Lemma 4 is not difficult anymore.

PROOF OF LEMMA 4 (SECTION 3.3):

Let P with $\|\langle \nu \rangle^l P\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon^{m+1}), \mathcal{D}(H_\varepsilon))} \lesssim 1$ for all $l \in \mathbb{N}_0$ be given. The similar proof for a P with $\|P \langle \nu \rangle^l\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon^m), \mathcal{H})} \lesssim 1$ for all $l \in \mathbb{N}_0$ will be omitted. We

start by proving $\|H_j P\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon^{m+1}), \mathcal{H})} \lesssim 1$ for $j = 0, 1, 2$. Exploiting that all the coefficients in H_j are bounded and have bounded derivatives we have

$$\begin{aligned} \|H_j P\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon^{m+1}), \mathcal{H})} &\lesssim \|H_j \langle \nu \rangle^{-16}\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon), \mathcal{H})} \\ &\lesssim \sum_{|\alpha|+|\beta| \leq 2} \|\langle \nu \rangle^{-8(|\alpha|+|\beta|)} \partial_n^\alpha \varepsilon^{|\beta|} \partial_x^\beta\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon), \mathcal{H})} \\ &\lesssim \|H_\varepsilon\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon), \mathcal{H})} = 1, \end{aligned} \quad (63)$$

where we made use of Lemma 10 iii) and Lemma 9 for the bound by H_ε . Now we set $\psi_P := P\psi$. By definition of H_ε

$$\begin{aligned} \langle \phi | H_\varepsilon \psi_P \rangle &= \langle \phi | D_\varepsilon M_\rho (-\varepsilon^2 \Delta_{\bar{g}} + V^\varepsilon) M_\rho^* D_\varepsilon^* \psi_P \rangle \\ &= \langle \phi | D_\varepsilon M_\rho (-\varepsilon^2 \Delta_{\bar{g}}) M_\rho^* D_\varepsilon^* \psi_P \rangle + \langle \phi | (V_c + D_\varepsilon^* W D_\varepsilon) \psi_P \rangle. \end{aligned} \quad (64)$$

Due to the assumption on P a Taylor expansion of $D_\varepsilon^* W D_\varepsilon$ in the fiber yields $D_\varepsilon^* W D_\varepsilon(q, \nu) P = (W(q, 0) + \varepsilon(\nabla_\nu^\vee W)(q, 0) + \frac{1}{2}\varepsilon^2(\nabla_{\nu, \nu}^\vee W)(q, 0)) P + \mathcal{O}(\varepsilon^3)$. Recalling that $V_0(q, \nu) = V_c(q, \nu) + W(q, 0)$ we find that

$$\begin{aligned} \langle \phi | (V_c + D_\varepsilon^* W D_\varepsilon) \psi_P \rangle &= \langle \phi | (V_0 + \varepsilon(\nabla_\nu^\vee W)(q, 0) + \frac{1}{2}\varepsilon^2(\nabla_{\nu, \nu}^\vee W)(q, 0)) \psi_P \rangle + \mathcal{O}(\varepsilon^3). \end{aligned} \quad (65)$$

The error estimate in Lemma 11 yields that $\|D_\varepsilon r_2 D_\varepsilon^* \langle \nu \rangle^{-1} \psi\| \lesssim \varepsilon \|\psi\|$ and thus $\|D_\varepsilon r_2 D_\varepsilon^* \psi_P\| \lesssim \varepsilon \|\psi_P\|$. By Lemma 1

$$\begin{aligned} &\langle \phi | D_\varepsilon M_\rho (-\varepsilon^2 \Delta_{\bar{g}}) M_\rho^* D_\varepsilon^* \psi_P \rangle \\ &= \int_{\mathcal{C}} \int_{N_q \mathcal{C}} \varepsilon^2 \bar{g} (dD_\varepsilon^* \phi^*, dD_\varepsilon^* \psi_P) d\nu d\mu + \varepsilon^2 \langle \phi | D_\varepsilon V_\rho D_\varepsilon^* \psi_P \rangle \\ &= \int_{\mathcal{C}} \int_{N_q \mathcal{C}} \varepsilon^2 \bar{g} (dD_\varepsilon^* \phi^*, dD_\varepsilon^* \psi_P) d\nu d\mu + \varepsilon^2 \langle \phi | V_{\text{geom}} \psi_P \rangle + \mathcal{O}(\varepsilon^3), \end{aligned} \quad (66)$$

where we used that V_{geom} does not depend on ν . Next we choose local coordinates as in Proposition 3 and insert the expansion for \bar{g} we obtained there into (66). We note that $\partial_{x^i} D_\varepsilon^* = D_\varepsilon^* \partial_{x^i}$ and $\partial_{n^\alpha} D_\varepsilon^* = \varepsilon^{-1} D_\varepsilon^* \partial_{n^\alpha}$.

$$\begin{aligned} &\int_{\Omega} \int_{N_q \mathcal{C}} \varepsilon^2 \bar{g} (dD_\varepsilon^* \phi^*, dD_\varepsilon^* \psi_P) d\nu d\mu \\ &= \int_{\Omega} \int_{\mathbb{R}^k} \varepsilon^2 \left((\partial_{x^i} + C_i^\alpha(q, n) \partial_{n^\alpha}) D_\varepsilon^* \phi^* \right) A^{ij}(q, n) (\partial_{x^j} + C_j^\beta(q, n) \partial_{n^\beta}) D_\varepsilon^* \psi_P \\ &\quad + \varepsilon^2 (\partial_{n^\alpha} D_\varepsilon^* \phi^*) B^{\alpha\beta}(q, n) \partial_{n^\beta} D_\varepsilon^* \psi_P dn d\mu + \mathcal{O}(\varepsilon^3) \\ &= \int_{\Omega} \int_{\mathbb{R}^k} \left((\varepsilon \partial_{x^i} + C_i^\alpha(q, \varepsilon n) \partial_{n^\alpha}) \phi^* \right) A^{ij}(q, \varepsilon n) (\varepsilon \partial_{x^j} + C_j^\beta(q, \varepsilon n) \partial_{n^\beta}) \psi_P \\ &\quad + (\partial_{n^\alpha} \phi^*) B^{\alpha\beta}(q, \varepsilon n) \partial_{n^\beta} \psi + \phi^* V_\varepsilon(q, n) \psi_P dn d\mu + \mathcal{O}(\varepsilon^3) \end{aligned} \quad (67)$$

because the bound on r_1 from Proposition 3 allows to conclude that the term containing $D_\varepsilon r_1 D_\varepsilon^*$ is of order ε^3 . To do so one bounds the partial derivatives by H_ε as in (63). After gathering the terms from (64) to (67) and plugging in the expressions from Proposition 3 the rest of the proof is just a matter of identifying ∇^\vee and ∇^h via (54) and (55). \square

4.3 Construction of the superadiabatic subspace P_ε

We search for a closed subspace $P_\varepsilon \mathcal{H} \subset \mathcal{H}$ and the corresponding orthogonal projection $P_\varepsilon \in \mathcal{L}(\mathcal{H})$ with

- i) $P_\varepsilon P_\varepsilon = P_\varepsilon$,
- ii) $[H_\varepsilon, P_\varepsilon] \chi(H_\varepsilon) = \mathcal{O}(\varepsilon^3)$

The former simply means that P_ε is a projection, while the latter says that $P_\varepsilon \mathcal{H}$ is invariant under the Hamiltonian H_ε upto errors of order ε^3 . We recall that U_0 and P_0 were defined by $U_0 \psi := \langle \varphi_0 | \psi \rangle_{\mathcal{H}_f}$ and $P_0 \psi := (U_0 \psi) \varphi_0$. Since $P_0^2 = P_0$ and $P_0 \mathcal{H}$ is invariant at least upto first order due to the slow variation of V_0 , we expect P_ε to have an expansion in ε starting with P_0 :

$$P_\varepsilon = P_0 + \varepsilon P_1 + \varepsilon^2 P_2 + \mathcal{O}(\varepsilon^3).$$

We first construct P_ε in a formal way not dealing with problems of boundedness. Afterwards we will show how to obtain a well-defined projector and the associated unitary U_ε .

We make the ansatz $P_1 := T_1^* P_0 + P_0 T_1$ with $T_1 : \mathcal{H} \rightarrow \mathcal{H}$ to be determined. Since P_0 is a spectral projection belonging to H_f , we know that $[H_f, P_0] = 0$, $[E_0, P_0] = 0$, and $H_f P_0 = E_0 P_0$. Lemma 4 yields that $H_0 = -\varepsilon^2 \Delta_h + H_f$. Assuming that $[P_1, -\varepsilon^2 \Delta_h + E_0] = \mathcal{O}(\varepsilon)$ we have

$$\begin{aligned} [H_\varepsilon, P_\varepsilon]/\varepsilon &= [H_0/\varepsilon + H_1, P_0 + \varepsilon P_1] + \mathcal{O}(\varepsilon) \\ &= [H_0/\varepsilon + H_1, P_0] + [H_0, P_1] + \mathcal{O}(\varepsilon) \\ &= [-\varepsilon \Delta_h + H_1, P_0] + [H_f - E_0, P_1] + \mathcal{O}(\varepsilon) \\ &= [-\varepsilon \Delta_h + H_1, P_0] + (H_f - E_0) T_1^* P_0 - P_0 T_1 (H_f - E_0) + \mathcal{O}(\varepsilon) \end{aligned}$$

We have to choose T_1 such that the first term vanishes. Observing that every term on the right hand side is off-diagonal with respect to P_0 , we may multiply with P_0 from the right and $1 - P_0$ from the left and vice versa to determine P_1 . This leads to

$$-(H_f - E_0)^{-1} (1 - P_0) ([-\varepsilon \Delta_h, P_0] + H_1) P_0 = (1 - P_0) T_1^* P_0 \quad (68)$$

and

$$-P_0 ([P_0, -\varepsilon\Delta_h] + H_1) (1 - P_0) (H_f - E_0)^{-1} = P_0 T_1 (1 - P_0), \quad (69)$$

where we have used that the operator $H_f - E_0$ is invertible on $(1 - P_0)\mathcal{H}_f$. In view of (68) and (69) we define T_1 by

$$T_1 := -P_0 ([P_0, -\varepsilon\Delta_h] + H_1) R_{H_f}(E_0) + R_{H_f}(E_0) ([-\varepsilon\Delta_h, P_0] + H_1) P_0 \quad (70)$$

with $R_{H_f}(E_0) = (H_f - E_0)^{-1}(1 - P_0) = (1 - P_0)(H_f - E_0)^{-1}$. T_1 is anti-symmetric so that $P^{(1)} := P_0 + \varepsilon P_1 = P_0 + \varepsilon(T_1^* P_0 + P_0 T_1)$ automatically satisfies the first condition for P_ε upto first order: Due to $P_0^2 = P_0$

$$\begin{aligned} P^{(1)} P^{(1)} &= P_0 + \varepsilon(T_1^* P_0 + P_0 T_1 + P_0(T_1^* + T_1)P_0) + \mathcal{O}(\varepsilon^2) \\ &= P_0 + \varepsilon(T_1^* P_0 + P_0 T_1) + \mathcal{O}(\varepsilon^2) \\ &= P^{(1)} + \mathcal{O}(\varepsilon^2). \end{aligned}$$

In order to derive the form of the second order correction, we make the ansatz $P_2 = T_1^* P_0 T_1 + T_2^* P_0 + P_0 T_2$ with some $T_2 : \mathcal{H} \rightarrow \mathcal{H}$. The anti-symmetric part of T_2 is determined analogously with T_1 just by calculating the commutator $[P_\varepsilon, H_\varepsilon]$ upto second order and inverting $H_f - E_0$. One ends up with

$$(T_2 - T_2^*)/2 = -P_0 ([P^{(1)}, H^{(2)}]/\varepsilon^2) R_{H_f}(E_0) + R_{H_f}(E_0) ([H^{(2)}, P^{(1)}]/\varepsilon^2) P_0$$

with $H^{(2)} := H_0 + \varepsilon H_1 + \varepsilon^2 H_2$. The symmetric part is again determined by the first condition for P_ε . Setting $P^{(2)} := P^{(1)} + \varepsilon^2 P_2$ we have

$$P^{(2)} P^{(2)} = P^{(2)} + \varepsilon^2 (P_0 T_1 T_1^* P_0 + P_0 (T_2^* + T_2) P_0) + \mathcal{O}(\varepsilon^3)$$

which forces $T_2 + T_2^* = -T_1 T_1^*$.

We note that T_1 includes a differential operator of second order (and T_2 even of fourth order) and will therefore not be bounded on the full Hilbert space and thus neither P_ε . This is related to the well-known fact that for a quadratic dispersion relation adiabatic decoupling breaks down for momenta tending to infinity. The problem can be circumvented by cutting off high energies in the right place, which was carried out by Sordani for the Born-Oppenheimer setting in [33] and by Tenuta and Teufel for a model of non-relativistic QED in [34].

To do so we fix $E < \infty$. Since H_ε is bounded from below, $E_- := \inf \sigma(H_\varepsilon)$ is finite. We choose $\chi_{E+1} \in C_0^\infty(\mathbb{R}, [0, 1])$ with $\chi_{E+1}|_{(E_- - 1, E+1]} \equiv 1$ and $\text{supp} \chi_{E+1} \subset (E_- - 2, E + 2]$. Then we define

$$\tilde{P}_\varepsilon := P^{(2)} - P_0 = \varepsilon(T_1^* P_0 + P_0 T_1) + \varepsilon^2(T_1^* P_0 T_1 + T_2^* P_0 + P_0 T_2) \quad (71)$$

and

$$P_\varepsilon^{\chi_{E+1}} := P_0 + \tilde{P}_\varepsilon \chi_{E+1}(H_\varepsilon) + \chi_{E+1}(H_\varepsilon) \tilde{P}_\varepsilon (1 - \chi_{E+1}(H_\varepsilon)) \quad (72)$$

with $\chi_{E+1}(H_\varepsilon)$ defined via the spectral theorem. We remark that $P_\varepsilon^{\chi_{E+1}}$ is symmetric.

We will show that $P_\varepsilon^{\chi_{E+1}} - P_0 = \mathcal{O}(\varepsilon)$ in the sense of bounded operators. Then for ε small enough a projector is obtained via the Riesz formula

$$P_\varepsilon := \frac{i}{2\pi} \oint_\Gamma (P_\varepsilon^{\chi_{E+1}} - z)^{-1} dz, \quad (73)$$

where $\Gamma = \{z \in \mathbb{C} \mid |z - 1| = 1/2\}$ is the positively oriented circle around 1. Following Nenciu and Sordani [25] we use the so-called Sz-Nagy formula

$$\tilde{U}_\varepsilon := (P_0 P_\varepsilon + (1 - P_0)(1 - P_\varepsilon)) (1 - (P_\varepsilon - P_0)^2)^{-1/2} \quad (74)$$

for a unitary mapping $\tilde{U}_\varepsilon : P_\varepsilon \mathcal{H} \rightarrow P_0 \mathcal{H}$. We now verify that P_ε and \tilde{U}_ε have indeed all the properties which we stated in Lemmas 2 & 5 and state here again for convenience:

Proposition 4 *Let $E < \infty$ and $\chi_{E+1} \in C^\infty(\mathbb{R}, [0, 1])$ with $\chi|_{(-\infty, E+1]} \equiv 1$ and $\text{supp } \chi_{E+1} \subset (-\infty, E+2]$.*

For a constraint energy band E_0 and $\varepsilon \ll 1$, P_ε defined by (71)-(73) is a bounded operator on \mathcal{H} and \tilde{U}_ε defined by (74) is unitary from $P_\varepsilon \mathcal{H}$ to $P_0 \mathcal{H}$. In particular, $P_\varepsilon = \tilde{U}_\varepsilon^ P_0 \tilde{U}_\varepsilon$.*

For each $m \in \mathbb{N}_0$ and $\chi \in C^\infty(\mathbb{R}, [0, 1])$ with $\text{supp } \chi \subset (-\infty, E+1]$ it holds $P_\varepsilon \in \mathcal{L}(\mathcal{D}(H_\varepsilon^m))$ and

$$\| [H_\varepsilon, P_\varepsilon] \|_{\mathcal{L}(\mathcal{D}(H_\varepsilon^{m+1}), \mathcal{D}(H_\varepsilon^m))} = \mathcal{O}(\varepsilon), \quad \| [H_\varepsilon, P_\varepsilon] \chi(H_\varepsilon) \|_{\mathcal{L}(\mathcal{H}, \mathcal{D}(H_\varepsilon^m))} = \mathcal{O}(\varepsilon^3).$$

Furthermore

- i) $\forall j, l \in \mathbb{N}_0 : \| \langle \nu \rangle^l P_\varepsilon \langle \nu \rangle^j \|_{\mathcal{L}(\mathcal{H})}, \| \langle \nu \rangle^l P_\varepsilon \langle \nu \rangle^j \|_{\mathcal{L}(\mathcal{D}(H_\varepsilon))} \lesssim 1$.*
- ii) $\forall j, l \in \mathbb{N}_0 : \| \langle \nu \rangle^l P_0 \langle \nu \rangle^j \|_{\mathcal{L}(\mathcal{D}(H_\varepsilon))} \lesssim 1, \| [-\varepsilon^2 \Delta_h, P_0] \|_{\mathcal{L}(\mathcal{D}(H_\varepsilon), \mathcal{H})} \lesssim \varepsilon$.*
- iii) There are $U_1^\varepsilon, U_2^\varepsilon \in \mathcal{L}(\mathcal{H}) \cap \mathcal{L}(\mathcal{D}(H_\varepsilon))$ with norms bounded independently of ε satisfying $P_0 U_1^\varepsilon P_0 = 0$ and $U_2^\varepsilon P_0 = P_0 U_2^\varepsilon P_0 = P_0 U_2^\varepsilon$ such that $\tilde{U}_\varepsilon = 1 + \varepsilon U_1^\varepsilon + \varepsilon^2 U_2^\varepsilon$. In particular, $\| \tilde{U}_\varepsilon - 1 \|_{\mathcal{L}(\mathcal{H})} = \mathcal{O}(\varepsilon)$.*
- iv) $\| P_0 U_1^\varepsilon \langle \nu \rangle^l \|_{\mathcal{L}(\mathcal{H})} \lesssim 1$ for all $l \in \mathbb{N}_0$.*
- v) For $B^\varepsilon := U_0^* U_\varepsilon \chi(H_\varepsilon)$ and all $u \in \{1, (U_1^\varepsilon)^*, (U_2^\varepsilon)^*\}$ it holds*

$$\| [-\varepsilon^2 \Delta_h + E_0, u P_0] B^\varepsilon \|_{\mathcal{L}(\mathcal{H})} = \mathcal{O}(\varepsilon). \quad (75)$$

vi) For $R_{H_f}(E_0) := (1 - P_0)(H_f - E_0)^{-1}(1 - P_0)$ it holds

$$\|U_1^{\varepsilon*} B^\varepsilon + R_{H_f}(E_0) ([-\varepsilon \Delta_h, P_0] + H_1) P_0 B^\varepsilon\|_{\mathcal{L}(\mathcal{H}, \mathcal{D}(H_\varepsilon))} = \mathcal{O}(\varepsilon).$$

vii) If $\varphi_0 \in C_b^m(\mathcal{C}, \mathcal{H}_f)$, there is $\lambda_0 \gtrsim 1$ with $\sup_q \|e^{\lambda_0 \langle \nu \rangle} \varphi_0(q)\|_{\mathcal{H}_f(q)} \lesssim 1$ and

$$\sup_q \|e^{\lambda_0 \langle \nu \rangle} \nabla_{\nu_1, \dots, \nu_l}^v \nabla_{\tau_1, \dots, \tau_m}^h \varphi_0(q)\|_{\mathcal{H}_f(q)} \lesssim 1$$

for all $\nu_1, \dots, \nu_l \in \Gamma_b(N\mathcal{C})$ and $\tau_1, \dots, \tau_m \in \Gamma_b(T\mathcal{C})$.

The proof relies substantially on the following decay properties of P_0 and the associated family of eigenfunctions.

Lemma 12 *Let $V_0 \in C_b^\infty(\mathcal{C}, C_b^\infty(N\mathcal{C}))$ and E_0 be a simple constraint energy band with family of projections P_0 as defined in Definition 3. Define $\nabla_{\tau_1}^h P_0 := [\nabla_{\tau_1}^h, P_0]$ and, inductively,*

$$\nabla_{\tau_1, \dots, \tau_m}^h P_0 := \nabla_{\tau_1}^h \nabla_{\tau_2, \dots, \tau_m}^h P_0 - \sum_{j=2}^m \nabla_{\tau_2, \dots, \tau_j}^h \nabla_{\tau_1, \dots, \tau_m}^h P_0$$

for arbitrary $\tau_1, \dots, \tau_m \in \Gamma(T\mathcal{C})$. For arbitrary $\nu_1, \dots, \nu_l \in \Gamma(N\mathcal{C})$ define $\nabla_{\nu_1, \dots, \nu_l}^v \nabla_{\tau_1, \dots, \tau_m}^h P_0 := [\nabla_{\nu_1}^v, \dots, [\nabla_{\nu_l}^v, \nabla_{\tau_1, \dots, \tau_m}^h P_0] \dots]$.

i) Then $E_0 \in C_b^\infty(\mathcal{C})$, $P_0 \in C_b^\infty(\mathcal{C}, \mathcal{L}(\mathcal{H}_f))$, and there is $\lambda_0 \gtrsim 1$ such that for all $\lambda \in [-\lambda_0, \lambda_0]$

$$\|e^{\lambda \langle \nu \rangle} R_{H_f}(E_0) e^{-\lambda \langle \nu \rangle}\|_{\mathcal{L}(\mathcal{H})} \lesssim 1$$

and

$$\|e^{\lambda \langle \nu \rangle} (\nabla_{\nu_1, \dots, \nu_l}^v \nabla_{\tau_1, \dots, \tau_m}^h P_0) e^{\lambda \langle \nu \rangle}\|_{\mathcal{L}(\mathcal{H})} \lesssim 1$$

for all $\nu_1, \dots, \nu_l \in \Gamma_b(N\mathcal{C})$ and $\tau_1, \dots, \tau_m \in \Gamma_b(T\mathcal{C})$.

Let φ_0 be a globally defined family of eigenfunctions corresponding to E_0 .

ii) If $\varphi_0 \in C_b^m(\mathcal{C}, \mathcal{H}_f)$, then $\varphi_0 \in C_b^m(\mathcal{C}, C_b^\infty(N\mathcal{C}))$. Furthermore

$$\sup_{q \in \mathcal{C}} \|e^{\lambda_0 \langle \nu \rangle} \varphi_0(q)\|_{\mathcal{H}_f(q)} \lesssim 1, \quad \sup_{q \in \mathcal{C}} \|e^{\lambda_0 \langle \nu \rangle} \nabla_{\nu_1, \dots, \nu_l}^v \nabla_{\tau_1, \dots, \tau_m}^h \varphi_0(q)\|_{\mathcal{H}_f(q)} \lesssim 1$$

for all $\nu_1, \dots, \nu_l \in \Gamma_b(N\mathcal{C})$ and $\tau_1, \dots, \tau_m \in \Gamma_b(T\mathcal{C})$.

iii) If \mathcal{C} is compact or contractable or if $E_0(q) = \inf \sigma(H_f(q))$ for all $q \in \mathcal{C}$, then φ_0 can be chosen such that $\varphi_0 \in C_b^\infty(\mathcal{C}, \mathcal{H}_f)$.

In addition, we need that the application of $\chi_{E+1}(H_\varepsilon)$ does not completely spoil the exponential decay. This is stated in the following lemma. Notice that we cannot expect it to preserve exponential decay in general, for we do not assume the cutoff energy E to lie below the continuous spectrum of H_ε !

Lemma 13 *Let $\chi \in C_0^\infty(\mathbb{R})$. For all $l \in \mathbb{N}$ and $m \in \{0, 1, 2, 3\}$*

$$\langle \nu \rangle^l \chi(H_\varepsilon) \langle \nu \rangle^{-l}, \langle \nu \rangle^{-l} \chi(H_\varepsilon) \langle \nu \rangle^l \in \mathcal{L}(\mathcal{H}, \mathcal{D}(H_\varepsilon^m))$$

with norms bounded independently of ε .

Now we give the proof of the proposition. Afterwards we take care of the two technical lemmas.

PROOF OF PROPOSITION 4:

We recall that we defined $E_- := \inf \sigma(H_\varepsilon)$. Let $\chi_E \in C_0^\infty(\mathbb{R}, [0, 1])$ with $\chi_E|_{[E_-, E]} \equiv 1$ and $\text{supp} \chi_E \subset [E_- - 1, E + 1]$. Then by the spectral theorem $\chi_E(H_\varepsilon)\chi(H_\varepsilon) = \chi(H_\varepsilon)$ and $\chi_{E+1}(H_\varepsilon)\chi_E(H_\varepsilon) = \chi_E(H_\varepsilon)$ for χ and χ_{E+1} as in the proposition.

The proof of the proposition will be divided into several steps. We drop all ε -subscripts except those of H_ε and write χ, χ_E , and χ_{E+1} for $\chi(H_\varepsilon), \chi_E(H_\varepsilon)$, and $\chi_{E+1}(H_\varepsilon)$ respectively. For convenience we set $\mathcal{D}(H_\varepsilon^0) := \mathcal{H}$.

We will often need that an operator $A \in \mathcal{L}(\mathcal{H})$ is in $\mathcal{L}(\mathcal{D}(H_\varepsilon^l, H_\varepsilon^m))$ for some $l, m \in \mathbb{N}_0$. The strategy to show that will always be to show that there are $l_1, l_2 \in \mathbb{N}$ with $l_1 + l_2 \leq 2l$ and

$$(-\varepsilon^2 \Delta_h - \Delta_v + V_\varepsilon)^m A \prec \langle \nu \rangle^{-4l_1 - 5l_2} (\nabla^v)^{l_1} (\varepsilon \nabla^h)^{l_2}. \quad (76)$$

Then we can use Lemma 9 to estimate:

$$\begin{aligned} \|H_\varepsilon^m A\psi\| + \|A\psi\| &\lesssim \|(-\varepsilon^2 \Delta_h - \Delta_v + V_\varepsilon)^m A\psi\| + \|\psi\| \\ &\lesssim \|\langle \nu \rangle^{-4l_1 - 5l_2} (\nabla^v)^{l_1} (\varepsilon \nabla^h)^{l_2} \psi\| + \|\psi\| \\ &\lesssim \|H_\varepsilon^{l_1} \psi\| + \|\psi\|, \end{aligned} \quad (77)$$

which yields the desired bound.

Step 1: $\exists \lambda_0 \gtrsim 1 \forall \lambda < \lambda_0, m \in \mathbb{N}_0 : \|e^{\lambda \langle \nu \rangle} P_0 e^{\lambda \langle \nu \rangle}\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon^m))} \lesssim 1$ and

$$\|e^{\lambda \langle \nu \rangle} [-\varepsilon^2 \Delta_h, P_0] e^{\lambda \langle \nu \rangle}\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon^{m+1}), \mathcal{D}(H_\varepsilon^m))} \lesssim \varepsilon.$$

Both statements hold true with $e^{\lambda \langle \nu \rangle}$ replaced by $\langle \nu \rangle^l$ for any $l \in \mathbb{N}_0$.

Let λ_0 be as given by Lemma 12. In order to obtain the estimate (76) for $A = e^{\lambda_0 \langle \nu \rangle} P_0 e^{\lambda_0 \langle \nu \rangle}$ we first commute all horizontal derivatives to the right and then the vertical ones. Using $V_0 \in C_b^\infty(\mathcal{C}, C_b^\infty(NC))$ and Lemma 9 we end up with terms of the form $e^{\lambda \langle \nu \rangle} (\nabla_{\nu_1, \dots, \nu_{m-l_1}}^v \nabla_{\tau_1, \dots, \tau_{m-l_2}}^h P_0) e^{\lambda \langle \nu \rangle} (\nabla^v)^{l_1} (\varepsilon \nabla^h)^{l_2}$ times a bounded function. By Lemma 12 we have

$$e^{\lambda \langle \nu \rangle} (\nabla_{\nu_1, \dots, \nu_{m-l_1}}^v \nabla_{\tau_1, \dots, \tau_{m-l_2}}^h P_0) e^{\lambda \langle \nu \rangle} (\nabla^v)^{l_1} (\varepsilon \nabla^h)^{l_2} \prec e^{-(\lambda_0 - \lambda) \langle \nu \rangle} (\nabla^v)^{l_1} (\varepsilon \nabla^h)^{l_2}$$

which implies (76) due to $\lambda < \lambda_0$. This yields the first claim of Step 1 via (77). The second claim can easily be proven in the same way. For the last claim it suffices to notice that $\|\langle \nu \rangle^l e^{-\lambda_0 \langle \nu \rangle}\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon^m))} \lesssim 1$ for all $l, m \in \mathbb{N}_0$, which is easy to verify.

Step 2: It holds $\forall \lambda < \lambda_0, m \in \mathbb{N}_0, i \in \{1, 2\}$:

$$\|e^{\lambda \langle \nu \rangle} T_i^* P_0 e^{\lambda \langle \nu \rangle}\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon^{m+i}), \mathcal{D}(H_\varepsilon^m))} \lesssim 1, \|e^{\lambda \langle \nu \rangle} P_0 T_i e^{\lambda \langle \nu \rangle}\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon^{m+i}), \mathcal{D}(H_\varepsilon^m))} \lesssim 1.$$

In particular, $\forall \lambda < \lambda_0, m \in \mathbb{N}_0$: $\|e^{\lambda \langle \nu \rangle} \tilde{P} e^{\lambda \langle \nu \rangle}\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon^{m+2}), \mathcal{D}(H_\varepsilon^m))} \lesssim \varepsilon$.

The last statement is an immediate consequence because

$$e^{\lambda \langle \nu \rangle} \tilde{P} e^{\lambda \langle \nu \rangle} = \varepsilon e^{\lambda \langle \nu \rangle} \left((T_1^* P_0 + P_0 T_1) + \varepsilon (T_1^* P_0 P_0 T_1 + T_2^* P_0 + P_0 T_2) \right) e^{\lambda \langle \nu \rangle}.$$

We carry out the proof of the first estimate only for $T_1^* P_0$. The same arguments work for the other terms. To obtain (76) for $A = e^{\lambda \langle \nu \rangle} T_1^* P_0 e^{\lambda \langle \nu \rangle}$ we again commute all derivatives in $(-\varepsilon^2 \Delta_h - \Delta_v + V_\varepsilon)^m$ and $T_1^* P_0$ to the right. In view of (70), the definition of T_1 , we have to compute the commutator of $R_{H_f}(E_0)$ with ∇^h and ∇^v . For arbitrary $\tau \in \Gamma_b(\mathcal{TC})$ it holds

$$\begin{aligned} [\nabla_\tau^h, R_{H_f}(E_0)] &= -(\nabla_\tau^h P_0) R_{H_f}(E_0) - R_{H_f}(E_0) (\nabla_\tau^h P_0) \\ &\quad - R_{H_f}(E_0) [\nabla_\tau^h, H_f - E_0] R_{H_f}(E_0). \end{aligned}$$

with $[\nabla_\tau^h, H_f - E_0] = (\nabla_\tau^h V_0 - \nabla_\tau E_0)$. The latter is bounded because of $V_0 \in C_b^\infty(\mathcal{C}, C_b^\infty(N_q \mathcal{C}))$ by assumption and $E_0 \in C_b^\infty(\mathcal{C})$ by Lemma 12. An analogous statement is true for ∇^v . Hence, we end up with all remaining derivatives on the right-hand side after a finite iteration. These are at most $2m + 2$. After exploiting that $\|e^{\lambda \langle \nu \rangle} R_{H_f}(E_0) e^{-\lambda \langle \nu \rangle}\|_{\mathcal{L}(\mathcal{H})} \lesssim 1$ by Lemma 12 we may obtain a bound by H_ε^{m+1} as in Step 1.

Step 3: $\forall m \in \mathbb{N}_0$: $\|P^{\chi_{E+1}}\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon^m))} \lesssim 1$ and

$$\forall j, l, \in \mathbb{N}_0, m \in \{0, 1\} : \|\langle \nu \rangle^j P^{\chi_{E+1}} \langle \nu \rangle^l\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon^m))} \lesssim 1.$$

We recall that

$$P^{\chi_{E+1}} = P_0 + \tilde{P} \chi_{E+1} + \chi_{E+1} \tilde{P} (1 - \chi_{E+1}).$$

Step 1 implies that $P_0 \in \mathcal{L}(\mathcal{D}(H_\varepsilon^m))$ for all $m \in \mathbb{N}_0$. So it suffices to bound the second and the third term to show that $P^{\chi_{E+1}} \in \mathcal{L}(\mathcal{D}(H_\varepsilon^m))$. Since H_ε is bounded from below and the support of χ_{E+1} is bounded from above, $\chi_{E+1} \in \mathcal{L}(\mathcal{H}, \mathcal{D}(H_\varepsilon^m))$ for every $m \in \mathbb{N}$. So the estimate for \tilde{P} obtained in

Step 2 implies the boundedness of the second term. By comparing them on the dense subset $\mathcal{D}(H_\varepsilon^2)$ we see that $\chi_{E+1}\tilde{P}$ is the adjoint of $\tilde{P}\chi_{E+1}$ and thus also bounded. This finally implies the boundedness of the third term, which establishes $P^{\chi_{E+1}} \in \mathcal{L}(\mathcal{D}(H_\varepsilon^m))$ for all $m \in \mathbb{N}_0$.

We now address the second claim. We fix λ with $0 < \lambda < \lambda_0$. Then

$$\begin{aligned} \langle \nu \rangle^j P^{\chi_{E+1}} \langle \nu \rangle^l &= \langle \nu \rangle^j P_0 \langle \nu \rangle^l + \langle \nu \rangle^j \tilde{P} \chi_{E+1} \langle \nu \rangle^l + \langle \nu \rangle^j \chi_{E+1} \tilde{P} (1 - \chi_{E+1}) \langle \nu \rangle^l \\ &= \langle \nu \rangle^j e^{-\lambda \langle \nu \rangle} (e^{\lambda \langle \nu \rangle} P_0 e^{\lambda \langle \nu \rangle}) e^{-\lambda \langle \nu \rangle} \langle \nu \rangle^l \\ &\quad + \langle \nu \rangle^j e^{-\lambda_0 \langle \nu \rangle} (e^{\lambda \langle \nu \rangle} \tilde{P} e^{\lambda \langle \nu \rangle}) (e^{-\lambda \langle \nu \rangle} \langle \nu \rangle^l) \langle \nu \rangle^{-l} \chi_{E+1} \langle \nu \rangle^l \\ &\quad + \langle \nu \rangle^j \chi_{E+1} \langle \nu \rangle^{-l} (\langle \nu \rangle^l e^{-\lambda \langle \nu \rangle}) (e^{\lambda \langle \nu \rangle} \tilde{P} e^{\lambda \langle \nu \rangle}) \\ &\quad \quad \times (e^{-\lambda \langle \nu \rangle} \langle \nu \rangle^l) \langle \nu \rangle^{-l} (1 - \chi_{E+1}) \langle \nu \rangle^l \end{aligned}$$

It is straight forward to see that $\|\langle \nu \rangle^j e^{-\lambda_0 \langle \nu \rangle}\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon^m))} \lesssim 1$ for all $j, m \in \mathbb{N}_0$. Therefore Step 1 yields the desired estimate for the first term. In addition, we know from Lemma 13 that $\|\langle \nu \rangle^{-l} \chi_{E+1} \langle \nu \rangle^l\|_{\mathcal{L}(\mathcal{H}, \mathcal{D}(H_\varepsilon^3))} \lesssim 1$. So Step 2 implies the desired estimate for the second term. Then it also follows for the third term by a standard adjoint argument.

Step 4: It holds $\forall m \in \mathbb{N}_0, i \in \{1, 2\}$

$$\begin{aligned} \|[T_i^* P_0, -\varepsilon^2 \Delta_h + E_0]\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon^{m+i+1}), \mathcal{D}(H_\varepsilon^m))} &= \mathcal{O}(\varepsilon), \\ \|[P_0 T_i, -\varepsilon^2 \Delta_h + E_0]\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon^{m+i+1}), \mathcal{D}(H_\varepsilon^m))} &= \mathcal{O}(\varepsilon). \end{aligned}$$

We again restrict to $T_1^* P_0$ assuring that the other proofs are similar. We note that E_0 commutes with all operators contained in $T_1^* P_0$ but the $\varepsilon \nabla^h$. Furthermore $\|[\varepsilon \nabla_\tau^h, E_0] P_0\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon^m))} = \varepsilon \|(\nabla_\tau E_0) P_0\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon^m))} = \mathcal{O}(\varepsilon)$ for all bounded τ by Lemma 12. So we easily see that $\|[T_1^* P_0, E_0]\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon^{m+2}), \mathcal{D}(H_\varepsilon^m))} = \mathcal{O}(\varepsilon)$.

We will obtain the claim of Step 4 for $T_1^* P_0$, if we are able to deduce that $\|[T_1^* P_0, -\varepsilon^2 \Delta_h]\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon^{m+2}), \mathcal{D}(H_\varepsilon^m))} = \mathcal{O}(\varepsilon)$. Again we aim at proving (76) by commuting all derivatives to the right. In Step 1 and Step 2 we have already treated the commutators of $-\varepsilon^2 \Delta_h$ with P_0 and $R_{H_f}(E_0)$. So it remains to disown showcuss $[\varepsilon \nabla_\tau^h, -\varepsilon^2 \Delta_h]$ which does not vanish in general! To do so we fix a covering $(\Omega_j)_{j \in \mathbb{N}}$ of \mathcal{C} as at the beginning of Section 4.1 and an arbitrary $j \in \mathbb{N}$. We choose an orthonormal frame $(\tau_i)_{i=1, \dots, d}$ in $T\Omega_j$. Using

that $\Delta_h = \sum_{i=1}^d \nabla_{\tau_i}^h \nabla_{\tau_i}^h$ we have

$$\begin{aligned}
[\varepsilon \nabla_{\tau}^h, -\varepsilon^2 \Delta_h] &= - \sum_{i=1}^d [\varepsilon \nabla_{\tau}^h, \varepsilon^2 \nabla_{\tau_i}^h \nabla_{\tau_i}^h] \\
&= - \sum_{i=1}^d (\varepsilon [\nabla_{\tau}^h, \varepsilon \nabla_{\tau_i}^h] \varepsilon \nabla_{\tau_i}^h + \varepsilon \nabla_{\tau_i}^h [\varepsilon \nabla_{\tau}^h, \varepsilon \nabla_{\tau_i}^h]) \\
&= -\varepsilon \sum_{i=1}^d \left(\varepsilon R^h(\tau, \tau_i) \varepsilon \nabla_{\tau_i}^h + \varepsilon \nabla_{[\tau, \tau_i]}^h \varepsilon \nabla_{\tau_i}^h \right. \\
&\quad \left. + \varepsilon \nabla_{\tau_i}^h \varepsilon R^h(\tau, \tau_i) + \varepsilon \nabla_{\tau_i}^h \varepsilon \nabla_{[\tau, \tau_i]}^h \right).
\end{aligned}$$

In view of Proposition 1 all these terms contain only two derivatives. So we have gained an ε because, although R^h and its derivatives grow linearly, we are able to bound the big bracket as required in (76) using the decay provided by P_0 . The estimate is independent of Ω_j because R^\perp is globally bounded due to our assumptions on the embedding of \mathcal{C} .

Step 5: For all $m \in \mathbb{N}_0$

$$\| [H_\varepsilon, P^{\chi_{E+1}}] \|_{\mathcal{L}(\mathcal{D}(H_\varepsilon^{m+1}), \mathcal{D}(H_\varepsilon^m))} = \mathcal{O}(\varepsilon), \quad \| [H_\varepsilon, P^{\chi_{E+1}}] \chi_E \|_{\mathcal{L}(\mathcal{H}, \mathcal{D}(H_\varepsilon^m))} = \mathcal{O}(\varepsilon^3).$$

We fix $m \in \mathbb{N}_0$. Due to the exponential decay obtained in Steps 1 & 2 for P_0 and \tilde{P} we may plug in the expansion of H_ε from Lemma 4 when deriving the stated estimates. The proof of Step 2 entails that $P^{\chi_{E+1}} - P_0$ is of order ε in $\mathcal{L}(\mathcal{D}(H_\varepsilon^m))$. Therefore

$$\begin{aligned}
\| [H_\varepsilon, P^{\chi_{E+1}}] \|_{\mathcal{L}(\mathcal{D}(H_\varepsilon^{m+1}), \mathcal{D}(H_\varepsilon^m))} &= \| [H_\varepsilon, P_0] \|_{\mathcal{L}(\mathcal{D}(H_\varepsilon^{m+1}), \mathcal{D}(H_\varepsilon^m))} + \mathcal{O}(\varepsilon) \\
&= \| [H_0, P_0] \|_{\mathcal{L}(\mathcal{D}(H_\varepsilon^{m+1}), \mathcal{D}(H_\varepsilon^m))} + \mathcal{O}(\varepsilon) \\
&= \| [\varepsilon^2 \Delta_h, P_0] \|_{\mathcal{L}(\mathcal{D}(H_\varepsilon^{m+1}), \mathcal{D}(H_\varepsilon^m))} + \mathcal{O}(\varepsilon) \\
&= \mathcal{O}(\varepsilon),
\end{aligned}$$

by Step 1. On the other hand we use $[H_\varepsilon, \chi_E] = 0$ and $(1 - \chi_{E+1})\chi_E = 0$ to obtain

$$\begin{aligned}
&\| [H_\varepsilon, P^{\chi_{E+1}}] \chi_E \|_{\mathcal{L}(\mathcal{H}, \mathcal{D}(H_\varepsilon^m))} \\
&= \| [H_\varepsilon, P^{(2)}] \chi_E \|_{\mathcal{L}(\mathcal{H}, \mathcal{D}(H_\varepsilon^m))} \\
&= \| [H_\varepsilon, P_0 + \tilde{P}] \chi_E \|_{\mathcal{L}(\mathcal{H}, \mathcal{D}(H_\varepsilon^m))} \\
&= \| [H_0 + \varepsilon H_1 + \varepsilon^2 H_2, P_0 + \tilde{P}] \chi_E \|_{\mathcal{L}(\mathcal{H}, \mathcal{D}(H_\varepsilon^m))} + \mathcal{O}(\varepsilon^3) = \mathcal{O}(\varepsilon^3),
\end{aligned}$$

where the last estimate follows from the construction of T_1 and T_2 (which were used to define \tilde{P}). To make precise the discussion at the beginning of

this subsection one uses Step 4 and once more the decay properties of P_0 and \tilde{P} to bound the error terms by H_ε^m for some $m \in \mathbb{N}$ as in (76) and (77).

Step 6: P, U are well-defined, $U|_{P\mathcal{H}}$ is unitary and $P \in \mathcal{L}(\mathcal{D}(H_\varepsilon^m))$ with

$$\|P - P_0\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon^m))} = \mathcal{O}(\varepsilon) \quad \forall m \in \mathbb{N}_0.$$

Since P_0 is a projector and $\|P^{\chi_{E+1}} - P_0\|_{\mathcal{L}(\mathcal{H})} = \mathcal{O}(\varepsilon)$, we have

$$\|(P^{\chi_{E+1}})^2 - P^{\chi_{E+1}}\|_{\mathcal{L}(\mathcal{H})} = \mathcal{O}(\varepsilon). \quad (78)$$

Now the spectral mapping theorem implies that there is a $C < \infty$ such that

$$\sigma(P^{\chi_{E+1}}) \subset [-C\varepsilon, C\varepsilon] \cup [1 - C\varepsilon, 1 + C\varepsilon].$$

Thus P is a well-defined bounded operator for $\varepsilon < 1/2C$. By the spectral theorem $P = \chi_{[1-C\varepsilon, 1+C\varepsilon]}(P^{\chi_{E+1}})$ and so $\|P - P^{\chi_{E+1}}\|_{\mathcal{L}(\mathcal{H})} = \mathcal{O}(\varepsilon)$. In particular, $P - P_0 = \mathcal{O}(\varepsilon)$ in $\mathcal{L}(\mathcal{H})$. Hence, $1 - (P - P_0)^2$ is positive and can be inverted. Therefore U is also a well-defined bounded operator with

$$U = U_0 (P + \mathcal{O}(\varepsilon^2)). \quad (79)$$

We set $S := (1 - (P - P_0)^2)^{-1/2}$. It is easy to verify that $[P, 1 - (P - P_0)^2] = 0 = [P_0, 1 - (P - P_0)^2]$ and thus $[P, S] = 0 = [P_0, S]$. The latter implies $\tilde{U}^* \tilde{U} = 1 = \tilde{U} \tilde{U}^*$. So \tilde{U} maps $P\mathcal{H}$ unitarily to $P_0\mathcal{H}$. Since U_0 is unitary when restricted to $P_0\mathcal{H}$, we see that $U = U_0 \tilde{U}$ is unitary when restricted to $P\mathcal{H}$.

The combination of (78) with Steps 3 and 5 immediately yields

$$\|(P^{\chi_{E+1}})^2 - P^{\chi_{E+1}}\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon^m))} = \mathcal{O}(\varepsilon).$$

for all $m \in \mathbb{N}_0$. So for $z \in \partial B_{1/2}(1)$ the resolvent $(P^{\chi_{E+1}} - z)^{-1}$ is an operator bounded independent of ε even on $\mathcal{D}(H_\varepsilon^m)$, which implies $P \in \mathcal{L}(\mathcal{D}(H_\varepsilon^m))$ in view of its definition. It follows as before that $P - P_0 = \mathcal{O}(\varepsilon)$ also in this space.

Step 7: $\|[H_\varepsilon, P]\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon^{m+1}), \mathcal{D}(H_\varepsilon^m))} = \mathcal{O}(\varepsilon)$ & $\|[H_\varepsilon, P] \chi_E\|_{\mathcal{L}(\mathcal{H}, \mathcal{D}(H_\varepsilon^m))} = \mathcal{O}(\varepsilon^3)$ for all $m \in \mathbb{N}_0$.

We observe that

$$[H_\varepsilon, P] = \frac{i}{2\pi} \oint_{\Gamma} (P^{\chi_{E+1}} - z)^{-1} [H_\varepsilon, P^{\chi_{E+1}}] (P^{\chi_{E+1}} - z)^{-1} dz.$$

Since we saw that $\|(P^{\chi_{E+1}} - z)^{-1}\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon^m))} \lesssim 1$ in the preceding step, the first estimate we claimed follows by inserting the result from Step 5. To deduce the second one we set $R_{P^{\chi_{E+1}}}(z) := (P^{\chi_{E+1}} - z)^{-1}$ and compute

$$\begin{aligned} [H_\varepsilon, P] \chi &= \frac{1}{2\pi} \oint_{\Gamma} R_{P^{\chi_{E+1}}}(z) [H_\varepsilon, P^{\chi_{E+1}}] R_{P^{\chi_{E+1}}}(z) \chi_E \chi dz \\ &= \frac{1}{2\pi} \oint_{\Gamma} R_{P^{\chi_{E+1}}}(z) [H_\varepsilon, P^{\chi_{E+1}}] \chi_E R_{P^{\chi_{E+1}}}(z) \chi \\ &\quad + R_{P^{\chi_{E+1}}}(z) [H_\varepsilon, P^{\chi_{E+1}}] [R_{P^{\chi_{E+1}}}(z), \chi_E] \chi dz. \end{aligned} \quad (80)$$

Furthermore

$$\begin{aligned} [R_{P^{\chi_{E+1}}}(z), \chi_E] \chi &= R_{P^{\chi_{E+1}}}(z) [P^{\chi_{E+1}}, \chi_E] R_{P^{\chi_{E+1}}}(z) \chi_E \chi \\ &= R_{P^{\chi_{E+1}}}(z) [P^{\chi_{E+1}}, \chi_E] \chi_E R_{P^{\chi_{E+1}}}(z) \chi \\ &\quad + R_{P^{\chi_{E+1}}}(z) [P^{\chi_{E+1}}, \chi_E] [R_{P^{\chi_{E+1}}}(z), \chi_E] \chi \\ &= R_{P^{\chi_{E+1}}}(z) [P^{\chi_{E+1}}, \chi_E] \chi_E R_{P^{\chi_{E+1}}}(z) \chi \\ &\quad + \left(R_{P^{\chi_{E+1}}}(z) [P^{\chi_{E+1}}, \chi_E] \right)^2 R_{P^{\chi_{E+1}}}(z) \chi. \end{aligned}$$

Since due to Step 5 we have $\|[P^{\chi_{E+1}}, H_\varepsilon]\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon^{m+1}), \mathcal{D}(H_\varepsilon^m))} = \mathcal{O}(\varepsilon)$ and $\|[P^{\chi_{E+1}}, H_\varepsilon] \chi_E\|_{\mathcal{L}(\mathcal{H}, \mathcal{D}(H_\varepsilon^m))} = \mathcal{O}(\varepsilon^3)$, Lemma 6 yields

$$\|[P^{\chi_{E+1}}, \chi_E]\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon^m), \mathcal{D}(H_\varepsilon^{m+1}))} = \mathcal{O}(\varepsilon), \quad \|[P^{\chi_{E+1}}, \chi_E] \chi_E\|_{\mathcal{L}(\mathcal{H}, \mathcal{D}(H_\varepsilon^m))} = \mathcal{O}(\varepsilon^3).$$

Applying these estimates, $\|R_{P^{\chi_{E+1}}}(z)\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon^m))} \lesssim 1$, and Step 5 to (80) we obtain $\|[H_\varepsilon, P] \chi(H_\varepsilon)\|_{\mathcal{L}(\mathcal{H}, \mathcal{D}(H_\varepsilon^m))} = \mathcal{O}(\varepsilon^3)$.

Step 8: $\forall j, l \in \mathbb{N}, m \in \{0, 1\} : \|\langle \nu \rangle^l P \langle \nu \rangle^j\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon^m))} \lesssim 1$.

This can be seen by applying the spectral calculus to $P^{\chi_{E+1}}$ which we know to be bounded and symmetric. Let $f : \mathbb{C} \rightarrow \mathbb{C}$ be defined by $f(z) := z$ and let $g : \mathbb{C} \rightarrow \{0, 1\}$ be the characteristic function of $B_{2/3}(1)$. Then due to (78) the spectral calculus implies that for ε small enough

$$\begin{aligned} P &= g(P^{\chi_{E+1}}) = f(P^{\chi_{E+1}}) (g/f^2)(P^{\chi_{E+1}}) f(P^{\chi_{E+1}}) \\ &= P^{\chi_{E+1}} (g/f^2)(P^{\chi_{E+1}}) P^{\chi_{E+1}}. \end{aligned}$$

We note that $(g/f^2)(P^{\chi_{E+1}}) \in \mathcal{L}(\mathcal{H})$ because $g \equiv 0$ in a neighborhood of zero. Since g/f^2 is holomorphic on $B_{1/2}(1)$, it holds

$$(g/f^2)(P^{\chi_{E+1}}) = \frac{i}{2\pi} \oint_{\partial B_{1/2}(1)} (g/f^2)(z) R_{P^{\chi_{E+1}}}(z) dz$$

by the Cauchy integral formula for bounded operators (see e.g. [12]). In the proof of Step 5 we saw that $R_{P^{\chi_{E+1}}}(z)$ is a bounded operator on $\mathcal{D}(H_\varepsilon)$ for $z \in \partial B_{1/2}(1)$, which implies that also $(g/f^2)(P^{\chi_{E+1}}) \in \mathcal{L}(\mathcal{D}(H_\varepsilon))$. Then Step 3 provides that $\|\langle \nu \rangle^l P \langle \nu \rangle^j\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon^m))} \lesssim 1$ for all $j, l \in \mathbb{N}$ and $m \in \{0, 1\}$, which yields the claim.

$$\text{Step 9: } \forall m \in \mathbb{N}_0 : \|(P - P^{\chi_{E+1}})\chi\|_{\mathcal{L}(\mathcal{H}, \mathcal{D}(H_\varepsilon^m))} = \mathcal{O}(\varepsilon^3)$$

Using that $T_1 = -T_1^*$ and $T_2 + T_2^* = -T_1 T_1^*$ as well as $P_0 T_1 P_0 = 0$ it is straight forward to verify that

$$\|\chi_E (P^{(2)} P^{(2)} - P^{(2)})\chi\|_{\mathcal{L}(\mathcal{H}, \mathcal{D}(H_\varepsilon^m))} = \mathcal{O}(\varepsilon^3). \quad (81)$$

Since $\|[P^{\chi_{E+1}}, H_\varepsilon]\chi\|_{\mathcal{L}(\mathcal{H}, \mathcal{D}(H_\varepsilon^{m-1}))} = \mathcal{O}(\varepsilon^3)$ by Step 5, Lemma 6 yields

$$\|[P^{\chi_{E+1}}, \chi_E]\chi\|_{\mathcal{L}(\mathcal{H}, \mathcal{D}(H_\varepsilon^m))} = \mathcal{O}(\varepsilon^3).$$

Recalling that $\|P^{\chi_{E+1}}\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon^m))}$ we have that in the norm of $\mathcal{L}(\mathcal{H}, \mathcal{D}(H_\varepsilon^m))$

$$\begin{aligned} & ((P^{\chi_{E+1}})^2 - P^{\chi_{E+1}})\chi \\ &= (P^{\chi_{E+1}} - 1)P^{\chi_{E+1}}\chi_E\chi \\ &= (P^{\chi_{E+1}} - 1)\chi_E P^{\chi_{E+1}}\chi + (P^{\chi_{E+1}} - 1)[P^{\chi_{E+1}}, \chi_E]\chi \\ &= \chi_E (P^{\chi_{E+1}} - 1)P^{\chi_{E+1}}\chi + [P^{\chi_{E+1}}, \chi_E]P^{\chi_{E+1}}\chi + \mathcal{O}(\varepsilon^3) \\ &= \chi_E (P^{(2)} - 1)P^{(2)}\chi + \mathcal{O}(\varepsilon^3) \\ &= \chi_E (P^{(2)} P^{(2)} - P^{(2)})\chi + \mathcal{O}(\varepsilon^3) \stackrel{(81)}{=} \mathcal{O}(\varepsilon^3). \end{aligned}$$

Since we know from the proof of Step 6 that $\|R_{P^{\chi_{E+1}}}(z)\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon^m))} \lesssim 1$ for z away from 0 and 1, the formula

$$P - P^{\chi_{E+1}} = \frac{1}{2\pi i} \oint_{\Gamma} \frac{R_{P^{\chi_{E+1}}}(z) + R_{P^{\chi_{E+1}}}(1-z)}{1-z} dz ((P^{\chi_{E+1}})^2 - P^{\chi_{E+1}}) \quad (82)$$

by Nenciu [24] implies that

$$\|(P - P^{\chi_{E+1}})\chi(H_\varepsilon)\|_{\mathcal{L}(\mathcal{H}, \mathcal{D}(H_\varepsilon^m))} = \mathcal{O}(\varepsilon^3). \quad (83)$$

Step 10: There are $U_1, U_2 \in \mathcal{L}(\mathcal{H}) \cap \mathcal{L}(\mathcal{D}(H_\varepsilon))$ with norms bounded independently of ε satisfying $P_0 U_1 P_0 = 0$ and $U_2 P_0 = P_0 U_2 P_0 = P_0 U_2$ such that $\tilde{U} = 1 + \varepsilon U_1 + \varepsilon^2 U_2$. In addition, $\|P_0 U_1^\varepsilon \langle \nu \rangle^l\|_{\mathcal{L}(\mathcal{H})} \lesssim 1$ for all $l \in \mathbb{N}_0$.

We define

$$U_1 := \varepsilon^{-1} (P_0 (\tilde{U} - 1) (1 - P_0) + (1 - P_0) (\tilde{U} - 1) P_0)$$

and

$$U_2 := \varepsilon^{-2}(P_0(\tilde{U} - 1)P_0 + (1 - P_0)(\tilde{U} - 1)(1 - P_0)).$$

Then $\tilde{U} = 1 + \varepsilon U_1 + \varepsilon^2 U_2$, $P_0 U_1 P_0 = 0$, and $P_0 U_2 = P_0 U_2 P_0 = U_2 P_0$ are clear. Next we fix $m \in \mathbb{N}_0$ and prove that $U_1 \in \mathcal{L}(\mathcal{D}(H_\varepsilon^m))$ with norm bounded independent of ε . The proof for U_2 is similar and will be omitted. We recall that

$$\tilde{U} = (P_0 P + (1 - P_0)(1 - P)) S$$

with $S := (1 - (P - P_0)^2)^{-1/2}$ and that we showed $[P, S] = 0 = [P_0, S]$ in Step 6. Therefore

$$\begin{aligned} U_1 &= \varepsilon^{-1}(P_0 \tilde{U}(1 - P_0) + (1 - P_0) \tilde{U} P_0) \\ &= \varepsilon^{-1} S (P_0 P (1 - P_0) + (1 - P_0)(1 - P) P_0) \\ &= \varepsilon^{-1} S (P_0(P - P_0)(1 - P_0) - (1 - P_0)(P - P_0) P_0). \end{aligned} \quad (84)$$

By Taylor expansion it holds

$$1 - S = \int_0^1 \frac{1}{2} (1 - s) (1 - s(P - P_0)^2)^{-\frac{3}{2}} ds (P - P_0)^2. \quad (85)$$

Let $h(x) := (1 - sx^2)^{-3/2}$ with $s \in [0, 1]$. h is holomorphic in $B_{1/2}(0)$. Due to Step 6 the spectrum of $P - P_0$ as an operator on $\mathcal{L}(\mathcal{D}(H_\varepsilon^m))$ is contained in $B_{1/4}(0)$ for ε small enough. Therefore $\|R_{P-P_0}(z)\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon^m))} \lesssim 1$ for $z \in \partial B_{1/2}(0)$ and $h(P - P_0) = \frac{i}{2\pi} \oint_{\partial B_{1/2}(0)} h(z) R_{P-P_0}(z) dz$. This allows us to conclude that the integral on the right hand side of (85) is an operator bounded independent of ε on $\mathcal{D}(H_\varepsilon^m)$. This implies that the whole right hand side is of order ε^2 in $\mathcal{L}(\mathcal{D}(H_\varepsilon^m))$ because $\|(P - P_0)^2\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon^m))} = \mathcal{O}(\varepsilon^2)$ by Step 6. So we get

$$U_1 = \varepsilon^{-1}(P_0(P - P_0)(1 - P_0) - (1 - P_0)(P - P_0)P_0) + \mathcal{O}(\varepsilon). \quad (86)$$

This yields the desired bound because $\|P - P_0\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon^m))} = \mathcal{O}(\varepsilon)$. We now turn to the last claim: Using $[S, P_0] = 0$ and $\|P_0 \langle \nu \rangle^l\|_{\mathcal{L}(\mathcal{H})} \lesssim 1$ due to Step 1 we obtain from (84) that

$$\begin{aligned} \|P_0 U_1^\varepsilon \langle \nu \rangle^l\|_{\mathcal{L}(\mathcal{H})} &= \|\varepsilon^{-1} S P_0 (P - P_0)(1 - P_0) \langle \nu \rangle^l\|_{\mathcal{L}(\mathcal{H})} \\ &\lesssim \|\varepsilon^{-1} (P - P_0) \langle \nu \rangle^l\|_{\mathcal{L}(\mathcal{H})} \end{aligned}$$

We note that the decay properties of P and P_0 themselves are not enough. Because of the ε^{-1} we really need to consider the difference. However, it holds $P - P_0 = (P - P^{\chi_{E+1}}) + (P^{\chi_{E+1}} - P_0)$ and via (82) the first difference

can be expressed by $(P^{\chi_{E+1}})^2 - P^{\chi_{E+1}}$. Looking at the proof of Step 3 we see that both differences consist only of terms that carry an ε with them and have the desired decay property.

Step 11: For $B := U_0^* U \chi(H_\varepsilon)$ and all $u \in \{1, U_1^*, U_2^*\}$

$$\| [-\varepsilon^2 \Delta_h + E_0, u P_0] B \|_{\mathcal{L}(\mathcal{H})} = \mathcal{O}(\varepsilon). \quad (87)$$

Again we restrict ourselves to the case $u = U_1^*$. It is obvious from the definition of U_1 in Step 10 that $[E_0, U_1^* P_0] = 0$. In view of (86), U_1 (and thus also U_1^*) contains, upto terms of order ε , a factor $P - P_0$. As long as we commute $(-\varepsilon^2 \Delta_h) P_0$ with the other factors, $P - P_0$ cancels the ε^{-1} in the definition of U_1 and the commutation yields the desired ε . Using that $B = P_0 \tilde{U} \chi = P_0 \chi + \mathcal{O}(\varepsilon)$ we have

$$\begin{aligned} [-\varepsilon^2 \Delta_h, U_1^* P_0] B &= [-\varepsilon^2 \Delta_h, U_1^* P_0] P_0 \chi + \mathcal{O}(\varepsilon) \\ &\stackrel{(86)}{=} [-\varepsilon^2 \Delta_h, \varepsilon^{-1} (1 - P_0) (P - P_0) P_0] P_0 \chi + \mathcal{O}(\varepsilon) \\ &= (1 - P_0) [-\varepsilon^2 \Delta_h, \varepsilon^{-1} (P - P_0)] P_0 \chi_E \chi + \mathcal{O}(\varepsilon) \\ &= (1 - P_0) [-\varepsilon^2 \Delta_h, \varepsilon^{-1} (P - P_0) \chi_E] P_0 \chi + \mathcal{O}(\varepsilon), \end{aligned}$$

The last step follows from $[(-\varepsilon^2 \Delta_h) P_0, \chi_E] \chi = \mathcal{O}(\varepsilon)$, which is implied by Lemma 6 because

$$\begin{aligned} [H_\varepsilon, (-\varepsilon^2 \Delta_h) P_0] \chi &= [-\varepsilon^2 \Delta_h + H_f, (-\varepsilon^2 \Delta_h) P_0] \chi + \mathcal{O}(\varepsilon) \\ &= [V_0, -\varepsilon^2 \Delta_h] P_0 \chi - \varepsilon^2 \Delta_h [-\varepsilon^2 \Delta_h, P_0] \chi + \mathcal{O}(\varepsilon) \\ &= \mathcal{O}(\varepsilon). \end{aligned}$$

Furthermore due to Step 9

$$\begin{aligned} (1 - P_0) [-\varepsilon^2 \Delta_h, \varepsilon^{-1} (P - P_0) \chi_E] P_0 \chi &= (1 - P_0) [-\varepsilon^2 \Delta_h, \varepsilon^{-1} (P^{\chi_{E+1}} - P_0) \chi_E] P_0 \chi + \mathcal{O}(\varepsilon^2) \\ &= (1 - P_0) [-\varepsilon^2 \Delta_h, (P_1 \chi_{E+1} + (1 - \chi_{E+1}) P_1 \chi_{E+1}) \chi_E] P_0 \chi + \mathcal{O}(\varepsilon) \\ &= (1 - P_0) [-\varepsilon^2 \Delta_h, (T_1^* P_0 + P_0 T_1) \chi_E] P_0 \chi + \mathcal{O}(\varepsilon). \end{aligned}$$

On the one hand,

$$(1 - P_0) [-\varepsilon^2 \Delta_h, P_0 T_1 \chi_E] = (1 - P_0) [-\varepsilon^2 \Delta_h, P_0] T_1 \chi_E = \mathcal{O}(\varepsilon)$$

by step 1. On the other hand,

$$\begin{aligned} (1 - P_0) [-\varepsilon^2 \Delta_h, T_1^* P_0 \chi_E] P_0 \chi &= (1 - P_0) T_1^* P_0 [(-\varepsilon^2 \Delta_h), \chi_E] P_0 \chi \\ &\quad + (1 - P_0) [-\varepsilon^2 \Delta_h, T_1^* P_0] \chi_E P_0 \chi + \mathcal{O}(\varepsilon) \\ &= (1 - P_0) T_1^* P_0 [(-\varepsilon^2 \Delta_h) P_0, \chi_E] \chi \\ &\quad + (1 - P_0) [-\varepsilon^2 \Delta_h, T_1^* P_0] \chi_E P_0 \chi + \mathcal{O}(\varepsilon) \\ &= \mathcal{O}(\varepsilon) \end{aligned}$$

due to Step 4 and the above argument that $[(-\varepsilon^2 \Delta_h) P_0, \chi_E] \chi = \mathcal{O}(\varepsilon)$.

Step 12: $\| (U_1^* + T_1^* P_0) B \|_{\mathcal{L}(\mathcal{H}, \mathcal{D}(H_\varepsilon^m))} = \mathcal{O}(\varepsilon)$ for all $m \in \mathbb{N}_0$.

All the following errors estimates will be in the norm of $\mathcal{L}(\mathcal{H}, \mathcal{D}(H_\varepsilon))$. Using again that $B = P_0 \tilde{U} \chi = P_0 \chi + \mathcal{O}(\varepsilon)$ as well as $\chi = \chi_E \chi$ we have that

$$\begin{aligned}
U_1^* B &= U_1^* P_0 \chi_E \chi + \mathcal{O}(\varepsilon) \\
&\stackrel{(86)}{=} \varepsilon^{-1} (1 - P_0) (P - P_0) P_0 \chi_E \chi + \mathcal{O}(\varepsilon) \\
&= \varepsilon^{-1} (1 - P_0) (P - P_0) \chi_E P_0 \chi + \mathcal{O}(\varepsilon) \\
&\stackrel{(83)}{=} \varepsilon^{-1} (1 - P_0) (P^{\chi_{E+1}} - P_0) \chi_E P_0 \chi + \mathcal{O}(\varepsilon) \\
&= (1 - P_0) (P_1 \chi_{E+1} + (1 - \chi_{E+1}) P_1 \chi_{E+1}) \chi_E P_0 \chi + \mathcal{O}(\varepsilon) \\
&= (1 - P_0) (T_1^* P_0 + P_0 T_1) \chi_E P_0 \chi + \mathcal{O}(\varepsilon) \\
&= T_1^* P_0 \chi + \mathcal{O}(\varepsilon) \\
&= T_1^* P_0 B + \mathcal{O}(\varepsilon)
\end{aligned}$$

because $(1 - P_0) T_1^* P_0 = T_1^* P_0$ by definition.

Step 13: If $\varphi_0 \in C_b^m(\mathcal{C}, \mathcal{H}_f)$, there is $\lambda_0 \gtrsim 1$ with $\sup_q \| e^{\lambda_0 \langle \nu \rangle} \varphi_0(q) \|_{\mathcal{H}_f(q)} \lesssim 1$ and $\sup_q \| e^{\lambda_0 \langle \nu \rangle} \nabla_{\nu_1, \dots, \nu_l}^v \nabla_{\tau_1, \dots, \tau_m}^h \varphi_0(q) \|_{\mathcal{H}_f(q)} \lesssim 1$ for all $\nu_1, \dots, \nu_l \in \Gamma_b(N\mathcal{C})$ and $\tau_1, \dots, \tau_m \in \Gamma_b(T\mathcal{C})$.

This is true by Lemma 12 ii). The results of Step 1 and Steps 6 to 13 together form Proposition 4. \square

PROOF OF LEMMA 12:

Because of $V_0 \in C_b^\infty(\mathcal{C}, C_b^\infty(N_q \mathcal{C}))$ and $[\nabla_\tau^h, \Delta_\nu] = 0$ for all τ due to Lemma 8 the mapping $q \mapsto (H_f(q) - z)^{-1}$ belongs to $C_b^\infty(\mathcal{C}, \mathcal{L}(\mathcal{H}_f))$. Since E_0 is a constraint energy band and thus separated, the projection $P_0(q)$ associated to $E_0(q)$ is given via the Riesz formula:

$$P_0(q) = -\frac{1}{2\pi} \oint_{\gamma(q)} (H_f(q) - z)^{-1} dz,$$

where $\gamma(q)$ is positively oriented closed curve encircling $E_0(q)$ once. It can be chosen independent of $q \in \mathcal{C}$ locally because the gap condition is uniform. Therefore $(H_f(\cdot) - z)^{-1} \in C_b^\infty(\mathcal{C}, \mathcal{L}(\mathcal{H}_f))$ entails $P_0 \in C_b^\infty(\mathcal{C}, \mathcal{L}(\mathcal{H}_f))$. This means in particular that $P_0 \mathcal{H}$ is a smooth subbundle. Therefore locally it is spanned by a smooth section φ_0 . By

$$E_0(q) P_0(q) = H_f(q) P_0(q) = -\frac{1}{2\pi} \oint_{\gamma(q)} z (H_f(q) - z)^{-1} dz$$

we see that also $E_0 P_0 \in C_b^\infty(\mathcal{C}, \mathcal{L}(\mathcal{H}_f))$. Then $E_0 = \text{tr}_{\mathcal{H}_f(\cdot)}(E_0 P_0) \in C_b^\infty(\mathcal{C})$ because covariant derivatives commute with taking the trace over smooth subbundles and derivatives of $E_0 P_0$ are trace-class operators. For example

$$\begin{aligned} \nabla_\tau \text{tr}(E_0 P_0) &= \nabla_\tau \text{tr}((E_0 P_0) P_0) \\ &= \text{tr}((\nabla_\tau^h E_0 P_0) P_0 + (E_0 P_0) \nabla_\tau^h P_0) \\ &= \text{tr}((\nabla_\tau^h E_0 P_0) P_0) + \text{tr}((E_0 P_0) \nabla_\tau^h P_0) < \infty \end{aligned}$$

for all $\tau \in \Gamma_b(T\mathcal{C})$ because P_0 and $E_0 P_0$ are trace-class and the product of a trace-class operator and a bounded operator is again trace-class (see [28], Theorem VI.19). The argument that higher derivatives of $E_0 P_0$ are trace-class is very similar.

Next we will prove the statement about invariance of exponential decay under the application of $R_{H_f}(E_0) := (1 - P_0)(H_f - E_0)^{-1}(1 - P_0)$. So let $\Psi \in \mathcal{H}_f$ be arbitrary. The claim is equivalent to showing that there is $\lambda_0 > 0$ such that for all $\lambda \in [-\lambda_0, \lambda_0]$

$$\Phi := e^{\lambda\langle\nu\rangle} R_{H_f}(E_0) e^{-\lambda\langle\nu\rangle} \Psi$$

satisfies $\|\Phi\|_{\mathcal{H}} \lesssim \sup_{q \in \mathcal{C}} \|\Psi\|_{\mathcal{H}}$. The latter immediately follows from

$$\|\Phi\|_{\mathcal{H}} \lesssim C \|e^{\lambda\langle\nu\rangle} (H_f - E_0) e^{-\lambda\langle\nu\rangle} \Phi\|_{\mathcal{H}} \quad (88)$$

because

$$\begin{aligned} \|e^{\lambda\langle\nu\rangle} (H_f - E_0) e^{-\lambda\langle\nu\rangle} \Phi\|_{\mathcal{H}} &= \|e^{\lambda\langle\nu\rangle} (1 - P_0) e^{-\lambda\langle\nu\rangle} \Psi\|_{\mathcal{H}} \\ &\leq \|\Psi\|_{\mathcal{H}} + \|e^{\lambda\langle\nu\rangle} P_0 e^{-\lambda\langle\nu\rangle}\|_{\mathcal{L}(\mathcal{H}_f)} \|\Psi\|_{\mathcal{H}} \\ &\lesssim \|\Psi\|_{\mathcal{H}}, \end{aligned}$$

where we used that E_0 is a constraint energy band by assumption. We now turn to (88). We note that by the Cauchy-Schwarz inequality it suffices to find a $\lambda_0 > 0$ such that for all $\lambda \in [-\lambda_0, \lambda_0]$

$$\langle \Phi | \Phi \rangle \lesssim |\text{Re} \langle \Phi | e^{\lambda\langle\nu\rangle} (H_f - E_0) e^{-\lambda\langle\nu\rangle} \Phi \rangle| \quad (89)$$

To derive (89) we start with the following useful estimate, which is easily obtained by commuting $H_f - E_0$ with $e^{-\lambda\langle\nu\rangle}$.

$$\begin{aligned} |\text{Re} \langle \Phi | e^{\lambda\langle\nu\rangle} (H_f - E_0) e^{-\lambda\langle\nu\rangle} \Phi \rangle| &= |\langle \Phi | (H_f - E_0) \Phi \rangle - \lambda^2 \langle \Phi | (|\nu|^2 / \langle \nu \rangle^2) \Phi \rangle| \\ &\geq |\langle \Phi | (H_f - E_0) \Phi \rangle| - \lambda^2 \langle \Phi | \Phi \rangle. \end{aligned}$$

Since E_0 is assumed to be a constraint energy band and thus separated by a gap, we have

$$\begin{aligned} |\langle \Phi | (H_f - E_0) \Phi \rangle| &= |\langle (1 - P_0) \Phi | (H_f - E_0) (1 - P_0) \Phi \rangle| \\ &\lesssim \langle (1 - P_0) \Phi | (1 - P_0) \Phi \rangle \\ &= (\langle \Phi | \Phi \rangle - \langle \Phi | P_0 \Phi \rangle). \end{aligned}$$

Since λ_0 can be chosen arbitrary small, we are left to show that $\langle \Phi | P_0 \Phi \rangle$ is strictly smaller than $\langle \Phi | \Phi \rangle$ independent of $\lambda \in [-\lambda_0, \lambda_0]$. We observe that

$$\begin{aligned} 1 = \operatorname{tr}_{\mathcal{H}_f(q)}(P_0^2(q)) &= \operatorname{tr}_{\mathcal{H}_f(q)}(e^{\Lambda_0\langle\nu\rangle} P_0(q) e^{\Lambda_0\langle\nu\rangle} e^{-\Lambda_0\langle\nu\rangle} P_0(q) e^{-\Lambda_0\langle\nu\rangle}) \\ &\leq \|e^{\Lambda_0\langle\nu\rangle} P_0(q) e^{\Lambda_0\langle\nu\rangle}\|_{\mathcal{H}_f(q)} \operatorname{tr}_{\mathcal{H}_f(q)}(e^{-\Lambda_0\langle\nu\rangle} P_0 e^{-\Lambda_0\langle\nu\rangle}). \end{aligned}$$

We know that $\|e^{\Lambda_0\langle\nu\rangle} P_0(q) e^{\Lambda_0\langle\nu\rangle}\|_{\mathcal{H}_f(q)} \leq C$ independent of $q \in \mathcal{C}$, since E_0 is a constraint energy band by assumption. Hence, for any λ with $\lambda \in [-\Lambda_0, \Lambda_0]$

$$\begin{aligned} \inf_q \operatorname{tr}_{\mathcal{H}_f(q)}(e^{-\lambda\langle\nu\rangle} P_0(q) e^{-\lambda\langle\nu\rangle}) &\geq \inf_q \operatorname{tr}_{\mathcal{H}_f(q)}(e^{-\Lambda_0\langle\nu\rangle} P_0(q) e^{-\Lambda_0\langle\nu\rangle}) \\ &\geq \left(\sup_q \|e^{\Lambda_0\langle\nu\rangle} P_0(q) e^{\Lambda_0\langle\nu\rangle}\|_{\mathcal{H}_f(q)} \right)^{-1} \geq C^{-1}. \end{aligned}$$

Since $P_0 e^{-\lambda\langle\nu\rangle} \Phi = 0$ by definition of Φ , we have

$$\begin{aligned} \langle \Phi | P_0 \Phi \rangle &= \langle \Phi | (P_0 - e^{-\lambda\langle\nu\rangle} P_0 e^{-\lambda\langle\nu\rangle}) \Phi \rangle \\ &\leq \sup_q \operatorname{tr}_{\mathcal{H}_f(q)}(P_0 - e^{-\lambda\langle\nu\rangle} P_0(q) e^{-\lambda\langle\nu\rangle}) \langle \Phi | \Phi \rangle \\ &\leq \left(\sup_q \operatorname{tr}_{\mathcal{H}_f(q)}(P_0) - \inf_q \operatorname{tr}_{\mathcal{H}_f(q)}(e^{-\lambda\langle\nu\rangle} P_0(q) e^{-\lambda\langle\nu\rangle}) \right) \langle \Phi | \Phi \rangle \\ &\leq (1 - C^{-1}) \langle \Phi | \Phi \rangle, \end{aligned}$$

which finishes the proof of (89).

For i) it remains to show that the derivatives of P_0 produce exponential decay. By definition P_0 satisfies

$$0 = (H_f - E_0)P_0 = -\Delta_v P_0 + V_0 P_0 - E_0 P_0. \quad (90)$$

Let $\tau_1, \dots, \tau_m \in \Gamma_b(\mathcal{TC})$ be arbitrary. To show that the derivatives of P_0 decay exponentially, we consider equations obtained by commuting the operator identity (90) with $\nabla_{\tau_1, \dots, \tau_m}^h$. Since Δ_v commutes with ∇^h by Lemma 8, this yields the following hierarchy of equations:

$$\begin{aligned} (H_f - E_0)(\nabla_{\tau_1}^h P_0) &= (\nabla_{\tau_1}^h E_0 - \nabla_{\tau_1}^h V_0) P_0, \\ (H_f - E_0)(\nabla_{\tau_1, \tau_2}^h P_0) &= (\nabla_{\tau_1, \tau_2}^h E_0 - \nabla_{\tau_1, \tau_2}^h V_0) P_0 + (\nabla_{\tau_2}^h E_0 - \nabla_{\tau_2}^h V_0)(\nabla_{\tau_1}^h P_0) \\ &\quad + (\nabla_{\tau_1}^h E_0 - \nabla_{\tau_1}^h V_0)(\nabla_{\tau_2}^h P_0), \end{aligned}$$

and analogous equations for higher and mixed derivatives. Applying the reduced resolvent $R_{H_f}(E_0)$ to both sides we obtain

$$(1 - P_0)(\nabla_{\tau_1}^h P_0) = R_{H_f}(E_0)(\nabla_{\tau_1}^h E_0 - \nabla_{\tau_1}^h V_0) P_0.$$

From $\|e^{\lambda_0\langle\nu\rangle}P_0e^{\lambda_0\langle\nu\rangle}\|_{\mathcal{L}(\mathcal{H})} \lesssim 1$ we can conclude that

$$\|e^{\lambda_0\langle\nu\rangle}(1-P_0)(\nabla_{\tau_1}^h P_0)e^{\lambda_0\langle\nu\rangle}\|_{\mathcal{L}(\mathcal{H})} \lesssim 1$$

because the derivatives of V_0 and E_0 are globally bounded and application of $R_{H_f}(E_0)$ preserves exponential decay as we have shown above. Inductively, we obtain that $\|e^{\lambda_0\langle\nu\rangle}(1-P_0)(\nabla_{\nu_1,\dots,\nu_l}^v \nabla_{\tau_1,\dots,\tau_m}^h P_0)e^{\lambda_0\langle\nu\rangle}\|_{\mathcal{L}(\mathcal{H})} \lesssim 1$. The same arguments yield $\|e^{\lambda_0\langle\nu\rangle}(\nabla_{\nu_1,\dots,\nu_l}^v \nabla_{\tau_1,\dots,\tau_m}^h P_0)(1-P_0)e^{\lambda_0\langle\nu\rangle}\|_{\mathcal{L}(\mathcal{H})} \lesssim 1$ when we start with $0 = P_0(H_f - E_0)$. The assumption $\|e^{\lambda_0\langle\nu\rangle}P_0e^{\lambda_0\langle\nu\rangle}\|_{\mathcal{L}(\mathcal{H})} \lesssim 1$ immediately implies $\|e^{\lambda_0\langle\nu\rangle}P_0(\nabla_{\nu_1,\dots,\nu_l}^v \nabla_{\tau_1,\dots,\tau_m}^h P_0)P_0e^{\lambda_0\langle\nu\rangle}\|_{\mathcal{L}(\mathcal{H})} \lesssim 1$.

We now turn to the second part of the lemma. By definition φ_0 satisfies

$$0 = (H_f - E_0)\varphi_0 = -\Delta_v\varphi_0 + V_0\varphi_0 - E_0\varphi_0. \quad (91)$$

for all $q \in \mathcal{C}$. Because of $V_0 \in C_b^\infty(\mathcal{C}, C_b^\infty(N_q\mathcal{C}))$ and $E_0 \in C_b^\infty(\mathcal{C})$ this is an elliptic equation with coefficients in $C_b^0(\mathcal{C}, C_b^\infty(N_q\mathcal{C}))$ on each fibre. So standard elliptic theory immediately implies $\varphi_0 \in C_b^0(\mathcal{C}, C_b^\infty(N_q\mathcal{C}))$. Due to the assumption that $\varphi_0 \in C_b^m(\mathcal{C}, \mathcal{H}_f(q))$ we may take horizontal derivatives of (91). Using that $[\Delta_v, \nabla_\tau^h]$ for all τ by Lemma 8 ii), we end up with the following equations

$$\begin{aligned} (H_f - E_0)\nabla_{\tau_1}^h\varphi_0 &= (\nabla_{\tau_1}E_0 - \nabla_{\tau_1}^hV_0)\varphi_0, \\ (H_f - E_0)\nabla_{\tau_1,\tau_2}^h\varphi_0 &= (\nabla_{\tau_1,\tau_2}E_0 - \nabla_{\tau_1,\tau_2}^hV_0)\varphi_0 + (\nabla_{\tau_1}E_0 - \nabla_{\tau_1}^hV_0)(\nabla_{\tau_2}^h\varphi_0) \\ &\quad + (\nabla_{\tau_2}E_0 - \nabla_{\tau_2}^hV_0)(\nabla_{\tau_1}^h\varphi_0), \end{aligned} \quad (92)$$

and analogous equations up to order m . Iteratively, we see that these are all elliptic equations with coefficients in $C_b^0(\mathcal{C}, C_b^\infty(N_q\mathcal{C}))$ on each fibre. Hence, we obtain $\varphi_0 \in C_b^0(\mathcal{C}, C_b^\infty(N_q\mathcal{C}))$. So we may take also vertical derivatives of the above hierarchy:

$$\begin{aligned} (H_f - E_0)\nabla_{\nu_1}^v\varphi_0 &= -(\nabla_{\nu_1}^vV_0)\varphi_0, \\ (H_f - E_0)\nabla_{\nu_1}^v\nabla_{\tau_1}^h\varphi_0 &= -(\nabla_{\nu_1}^v\nabla_{\tau_1}^hV_0)\varphi_0 - (\nabla_{\nu_1}^vV_0)(\nabla_{\tau_1}^h\varphi_0) \\ &\quad + (\nabla_{\tau_1}E_0 - \nabla_{\tau_1}^hV_0)\nabla_{\nu_1}^v\varphi_0 \end{aligned} \quad (93)$$

and so on. Since E_0 is assumed to be a constraint energy band, we have that

$$\|e^{\Lambda_0\langle\nu\rangle}\varphi_0\langle e^{\Lambda_0\langle\nu\rangle}\varphi_0|\psi\rangle_{\mathcal{H}_f(q)}\|_{\mathcal{H}_f(q)} = \|e^{\Lambda_0\langle\nu\rangle}P_0e^{\Lambda_0\langle\nu\rangle}\psi\|_{\mathcal{H}_f(q)} \lesssim \|\psi\|_{\mathcal{H}_f(q)}$$

with a constant independent of q . Choosing $\psi = e^{-\Lambda_0\langle\nu\rangle}\varphi_0$ and taking the supremum over $q \in \mathcal{C}$ we obtain the desired exponential decay of φ_0 . Because

of $V_0 \in C_b^\infty(\mathcal{C}, C_b^\infty(N_q\mathcal{C}))$ and $E_0 \in C_b^\infty(\mathcal{C})$ also the right-hand sides of (92) and (93) decay exponentially. By i) an application of $R_{H_f}(E_0)$ preserves exponential decay. So we may conclude that the φ_0 -orthogonal parts of $\nabla_{\tau_1}^h \varphi_0$ and $\nabla_{\nu_1}^v \varphi_0$ decay exponentially. Together with the exponential decay of φ_0 this entails the desired exponential decay of $\nabla_{\tau_1}^h \varphi_0$ and $\nabla_{\nu_1}^v \varphi_0$. This argument can now easily be iterated for the higher derivatives.

Finally we turn to iii). We consider a normalized trivializing section φ_0 , in particular $\sup_{q \in \mathcal{C}} \|\varphi_0\|_{\mathcal{H}_f}$ is globally bounded. The smoothness of the section φ_0 in $P_0\mathcal{H}$ is granted from the abstract existence argument of a global section via Chern classes. In order to see that it is also smooth in $(1 - P_0)\mathcal{H}$, one applies $R_{H_f}(E_0)$ to the equations (92), which can be justified by an approximation argument. Hence, we only need to show boundedness of all the derivatives. If \mathcal{C} is compact, this is clear.

If \mathcal{C} is contractible, all bundles over \mathcal{C} are trivializable. In particular, already the real eigenspace bundle $P_0\mathcal{H}$ has a global smooth trivializing section φ_0 . We choose a covering of \mathcal{C} by geodesic balls of fixed diameter and take an arbitrary one of them called Ω . We fix $q_0 \in \Omega$ and choose geodesic coordinates $(x^i)_{i=1, \dots, d}$ and bundle coordinates $(n^\alpha)_{\alpha=1, \dots, k}$ with respect to an orthonormal trivializing frame $\{\nu_\alpha\}_\alpha$ over Ω . Hereby $\{\nu_\alpha\}_\alpha$ is chosen such that $\Gamma_{i\beta}^\alpha$ is bounded and smooth which is possible due to our assumptions on the embedding of \mathcal{C} . Since φ_0 is the only normalized element of the real $P_0\mathcal{H}$, we have that

$$\varphi_0(q) = \frac{P_0(q)\varphi_0(q_0)}{\|P_0(q)\varphi_0(q_0)\|} \quad (94)$$

for q close to q_0 (which only makes sense in coordinates). Therefore we can split up $\nabla_{\partial_{x^i}}^h \varphi_0$ into terms depending on $\nabla_{\partial_{x^i}}^h P_0$, which are bounded due to i), and terms depending on $\nabla_{\partial_{x^i}}^h (\varphi_0(q_0))$. In view of the coordinate expression $\nabla_{\partial_{x^i}}^h = \partial_{x^i} - \Gamma_{i\beta}^\alpha n^\beta \partial_{n^\alpha}$ the latter is equal to $-\Gamma_{i\beta}^\alpha n^\beta \partial_{n^\alpha} \varphi_0(q_0)$. We already know that $\varphi_0 \in C_b^0(\mathcal{C}, \mathcal{H}_f(q))$. By ii) this implies $\varphi_0 \in C_b^0(\mathcal{C}, C_b^\infty(N_q\mathcal{C}))$ with $\sup_q \|e^{\lambda_0 \langle \nu \rangle} \varphi_0\| \lesssim 1$. Hence, we have that $-\Gamma_{i\beta}^\alpha n^\beta \partial_{n^\alpha} \varphi_0(q_0)$ is bounded. Noticing that all the bounds are independent of Ω due to the bounded geometry of \mathcal{C} , we obtain that $\varphi_0 \in C_b^1(\mathcal{C}, \mathcal{H}_f(q))$. Now we can inductively make use of (94) and ii) to obtain $\varphi_0 \in C_b^\infty(\mathcal{C}, \mathcal{H}_f(q))$.

If $E_0 = \inf \sigma(H_f(q))$ for all $q \in \mathcal{C}$, again the real eigenspace bundle is already trivializable. To see this we note that the groundstate of a real Schrödinger operator can always be chosen strictly positive, which defines an orientation on the real eigenspace bundle. A real line bundle with an orientation is trivializable. So we may argue as in the case of a contractable \mathcal{C} to obtain that the derivatives are globally bounded. \square

PROOF OF LEMMA 13:

Let $l \in \mathbb{Z}$. We fix $m \in \{1, 2, 3\}$ and $z_1, \dots, z_m \in \mathbb{C} \setminus \mathbb{R} \cap \text{supp } \chi \times [-1, 1]$. We claim that there is a $c > 0$ independent of ε and the z_i such that

$$\left\| \prod_{i=1}^m (H_\varepsilon - z_i) \langle \lambda \nu \rangle^l \prod_{j=1}^m R_{H_\varepsilon}(z_j) \langle \nu \rangle^{-l} \right\|_{\mathcal{L}(\mathcal{H})} \leq 2 \quad (95)$$

for $\lambda := \min \left\{ 1, \frac{c \prod_{i=1}^m |\text{Im} z_i|}{1 + \prod_{j=1}^m (|z_j| + |\text{Im} z_j|)} \right\} > 0$.

To prove this we set $\Phi := \prod_{i=1}^m (H_\varepsilon - z_i) \langle \lambda \nu \rangle^l \prod_{j=1}^m R_{H_\varepsilon}(z_j) \langle \nu \rangle^{-l} \Psi$ for $\Psi \in \mathcal{H}$ and aim to show that $\|\Psi\| \geq \|\Phi\|/2$. Because of $\lambda \leq 1$ we have that

$$\begin{aligned} \|\Psi\| &= \left\| \langle \nu \rangle^l \prod_{j=1}^m (H_\varepsilon - z_j) \langle \lambda \nu \rangle^{-l} \prod_{i=1}^m R_{H_\varepsilon}(z_j) \Phi \right\| \\ &\geq \left\| \langle \lambda \nu \rangle^l \prod_{j=1}^m (H_\varepsilon - z_j) \langle \lambda \nu \rangle^{-l} \prod_{i=1}^m R_{H_\varepsilon}(z_j) \Phi \right\| \\ &\geq \|\Phi\| - \left\| \langle \lambda \nu \rangle^l \left[\prod_{j=1}^m (H_\varepsilon - z_j), \langle \lambda \nu \rangle^{-l} \right] \prod_{i=1}^m R_{H_\varepsilon}(z_j) \Phi \right\| \end{aligned}$$

All terms in the commutator carry a positive power of λ because at least one derivative has to hit $\langle \lambda \nu \rangle^{-l}$. Because of $\lambda \leq 1$ positive powers of λ are bounded by λ . Using that $|z_i|$ is uniformly bounded and Lemma 9 iii) we have that there is a $C < \infty$ independent of ε, λ and the z_i 's with

$$\begin{aligned} \|\Psi\| &\geq \|\Phi\| - C\lambda \left(\left\| H_\varepsilon^m \prod_{j=1}^m R_{H_\varepsilon}(z_j) \Phi \right\| + \left\| \prod_{j=1}^m R_{H_\varepsilon}(z_j) \Phi \right\| \right) \\ &= \|\Phi\| - C\lambda \left\| \prod_{j=1}^m H_\varepsilon R_{H_\varepsilon}(z_j) \Phi \right\| - C\lambda \left\| \prod_{j=1}^m R_{H_\varepsilon}(z_j) \Phi \right\| \\ &\geq \|\Phi\| - C\lambda \prod_{j=1}^m \left(1 + \frac{|z_j|}{|\text{Im} z_j|} \right) \|\Phi\| - C\lambda \prod_{j=1}^m |\text{Im} z_j|^{-1} \|\Phi\| \\ &\geq \|\Phi\| - C\lambda \frac{1 + \prod_{j=1}^m (|z_j| + |\text{Im} z_j|)}{\prod_{i=1}^m |\text{Im} z_i|} \|\Phi\| \\ &\geq \|\Phi\|/2 \end{aligned}$$

for $\lambda \leq \frac{(2C)^{-1} \prod_{i=1}^m |\text{Im} z_i|}{1 + \prod_{j=1}^m (|z_j| + |\text{Im} z_j|)}$. This yields (95).

Now we make use of the Helffer-Sjöstrand formula again. We recall from the proof of Lemma 6 that it says that

$$f(H_\varepsilon) = \frac{1}{\pi} \int_{\mathbb{C}} \partial_{\bar{z}} \tilde{f}(z) R_{H_\varepsilon}(z) dz,$$

where \tilde{f} is an arbitrary almost analytic extension of f . As before by dz we mean the usual volume on \mathbb{C} . By assumption χ is non-negative. So by the spectral theorem we have $\chi(H_\varepsilon) = \prod_{i=1}^m \chi^{1/m}(H_\varepsilon)$. We choose an almost analytic extension of $\chi^{1/m}$ such that $K := \text{supp } \widetilde{\chi^{1/m}} \subset \text{supp } \chi \times [-1, 1]$, i.e. the volume of K is independent of ε , and

$$|\partial_{\bar{z}} \widetilde{\chi^{1/m}}(z)| = \mathcal{O}(|\text{Im} z|^{l+1}). \quad (96)$$

Then by the Helffer-Sjöstrand formula

$$\chi(H_\varepsilon) = \frac{1}{\pi^m} \int_{\mathbb{C}^m} \prod_{i=1}^m \partial_{\bar{z}} \widetilde{\chi^{1/m}}(z_i) \prod_{i=1}^m R_{H_\varepsilon}(z_i) dz_1 \dots dz_m.$$

We will now combine (95) and (96) to obtain the claimed estimate.

$$\begin{aligned} & |\langle \nu \rangle^l \chi(H_\varepsilon) \langle \nu \rangle^{-l} \Psi| \\ &= \left| \frac{1}{\pi^m} \int_{\mathbb{C}^m} \prod_{i=1}^m \partial_{\bar{z}} \widetilde{\chi^{1/m}}(z_i) \langle \nu \rangle^l \langle \lambda \nu \rangle^{-l} \langle \lambda \nu \rangle^l \prod_{i=1}^m R_{H_\varepsilon}(z_i) \langle \nu \rangle^{-l} \Psi dz_1 \dots dz_m \right| \\ &\stackrel{(96)}{\lesssim} \int_{K^m} \prod_{i=1}^m |\text{Im} z_i| \left| \langle \lambda \nu \rangle^l \prod_{i=1}^m R_{H_\varepsilon}(z_i) \langle \nu \rangle^{-l} \Psi \right| dz_1 \dots dz_m \end{aligned}$$

where we used that $\langle \nu \rangle^l \langle \lambda \nu \rangle^{-l} \lesssim \lambda^{-l} \sim \prod_{i=1}^m |\text{Im} z_i|^{-l}$ for small $|\text{Im} z_i|$. Therefore

$$\begin{aligned} & \left\| \langle \nu \rangle^l \chi(H_\varepsilon) \langle \nu \rangle^{-l} \Psi \right\|_{\mathcal{D}(H_\varepsilon^m)} \\ &\lesssim \left\| \int_{K^m} \prod_{i=1}^m |\text{Im} z_i| \left| \langle \lambda \nu \rangle^l \prod_{i=1}^m R_{H_\varepsilon}(z_i) \langle \nu \rangle^{-l} \Psi \right| dz_1 \dots dz_m \right\|_{\mathcal{D}(H_\varepsilon^m)} \\ &= \left\| \int_{K^m} \prod_{i=1}^m |\text{Im} z_i| \left| \prod_{i=1}^m R_{H_\varepsilon}(z_i) \prod_{i=1}^m (H_\varepsilon - z_i) \langle \lambda \nu \rangle^l \right. \right. \\ &\quad \left. \left. \times \prod_{i=1}^m R_{H_\varepsilon}(z_i) \langle \nu \rangle^{-l} \Psi \right| dz_1 \dots dz_m \right\|_{\mathcal{D}(H_\varepsilon^m)} \\ &\leq \int_{K^m} \prod_{i=1}^m |\text{Im} z_i| \prod_{i=1}^m \|R_{H_\varepsilon}(z_i)\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon^{m-i}), \mathcal{D}(H_\varepsilon^{m-i+1}))} \\ &\quad \times \left\| \prod_{i=1}^m (H_\varepsilon - z_i) \langle \lambda \nu \rangle^l \prod_{i=1}^m R_{H_\varepsilon}(z_i) \langle \nu \rangle^{-l} \Psi \right\|_{\mathcal{H}} dz_1 \dots dz_m \\ &\stackrel{(95)}{\lesssim} \|\Psi\|_{\mathcal{H}}, \end{aligned}$$

by the resolvent estimate (47). Hence, $\langle \nu \rangle^l \chi(H_\varepsilon) \langle \nu \rangle^{-l} \in \mathcal{L}(\mathcal{H}, \mathcal{D}(H_\varepsilon^m))$ with norm independent of ε for $m \in \{1, 2, 3\}$. The same holds for $\langle \lambda \nu \rangle^{-l} \chi(H_\varepsilon) \langle \nu \rangle^l$ which is easily seen by a similar proof. The case $m = 0$ is a trivial consequence of $m = 1$. \square

Appendix

Manifolds of bounded geometry

Here we explain shortly the notion of bounded geometry which provides the natural framework for this paper. More on the subject can be found in [32].

Definition 5 *Let (\mathcal{M}, g) be a Riemannian manifold and let r_q denote the injectivity radius at $q \in \mathcal{M}$. Set $r_{\mathcal{M}} := \inf_{q \in \mathcal{M}} r_q$. (\mathcal{M}, g) is said to be of bounded geometry if $r_{\mathcal{M}} > 0$ and every covariant derivative of the Riemann tensor \mathcal{R} is bounded, i.e.*

$$\forall m \in \mathbb{N} \quad \exists C_m < \infty : \quad g(\nabla^m \mathcal{R}, \nabla^m \mathcal{R}) \leq C_m.$$

Here ∇ is the Levi-Civita connection on (\mathcal{M}, g) and g is extended to the tensor bundles $T_m^l \mathcal{M}$ for all $l, m \in \mathbb{N}$ in the canonical way.

The definition of the Riemann tensor is given below. We note that $r_{\mathcal{M}} > 0$ implies completeness of \mathcal{M} . The second condition is equivalent to postulating that every transition function between an arbitrary pair of geodesic coordinate charts has bounded derivatives upto any order.

The geometry of submanifolds

We recall here some standard concepts from Riemannian geometry. We especially focus on the generalization of the usual tensors to submanifolds with codimension higher than one, which are omitted in some textbooks. For further information see [10].

First, however, we give the definitions of the inner curvature tensors we use because they vary in the literature. We note that they contain statements about linearity and independence of basis that are not proved here! In the following we denote by $\Gamma(\mathcal{E})$ the set of all smooth sections of a bundle \mathcal{E} and by $\mathcal{T}_m^l(\mathcal{M})$ the set of all smooth (l, m) -tensor fields over a manifold \mathcal{M} .

Definition 6 *Let (\mathcal{A}, \bar{g}) be a Riemannian manifold with Levi-Civita connection $\bar{\nabla}$. Let $\tau_1, \tau_2, \tau_3, \tau_4 \in \Gamma(T\mathcal{A})$.*

i) The curvature mapping $\bar{\mathbf{R}} : \Gamma(T\mathcal{A}) \times \Gamma(T\mathcal{A}) \rightarrow \mathcal{T}_1^1(\mathcal{A})$ is given by

$$\bar{\mathbf{R}}(\tau_1, \tau_2) \tau_3 := \bar{\nabla}_{\tau_1} \bar{\nabla}_{\tau_2} \tau_3 - \bar{\nabla}_{\tau_2} \bar{\nabla}_{\tau_1} \tau_3 - \bar{\nabla}_{[\tau_1, \tau_2]} \tau_3.$$

ii) The Riemann tensor $\bar{\mathcal{R}} \in \mathcal{T}_4^0(\mathcal{A})$ is given by

$$\bar{\mathcal{R}}(\tau_1, \tau_2, \tau_3, \tau_4) := \bar{g}(\tau_1, \bar{\mathbf{R}}(\tau_3, \tau_4) \tau_2).$$

iii) The Ricci tensor $\bar{\mathbf{Ric}} \in \mathcal{T}_2^0(\mathcal{A})$ is given by

$$\bar{\mathbf{Ric}}(\tau_1, \tau_2) := \text{tr}_{\mathcal{A}} \bar{\mathbf{R}}(\cdot, \tau_1) \tau_2.$$

iv) The scalar curvature $\bar{\kappa} : \mathcal{A} \rightarrow \mathbb{R}$ is given by

$$\bar{\kappa} := \text{tr}_{\mathcal{A}} \bar{\mathbf{Ric}}.$$

Here $\text{tr}_{\mathcal{A}} t$ means contracting the tensor t by an arbitrary orthonormal basis of $T\mathcal{A}$.

Remark 3 The dependence on vector fields of $\bar{\mathbf{R}}$, $\bar{\mathcal{R}}$, and $\bar{\mathbf{Ric}}$ can be lifted to the cotangent bundle TC^* via the metric \bar{g} . The resulting objects are denoted by the same letters throughout this paper. The same holds for all the objects defined below.

Of course, all these objects can also be defined for a submanifold once a connection has been chosen. There is a canonical choice given by the induced connection.

Definition 7 Let $\mathcal{C} \subset \mathcal{A}$ be a submanifold with induced metric g . Denote by TC and NC the tangent and the normal bundle of \mathcal{C} . Let $\tau_1, \tau_2, \tau_3 \in \Gamma(TC)$.

i) We define ∇ to be the induced connection on \mathcal{C} given via

$$\nabla_{\tau_1} \tau_2 := P_T \bar{\nabla}_{\tau_1} \tau_2,$$

where τ_1, τ_2 are canonically lifted to $T\mathcal{A} = TC \times NC$ and P_T denotes the projection onto the first component of the decomposition. The projection onto the second component of the decomposition will be denoted by P_{\perp} .

ii) The induced curvature mapping $\mathbf{R} : \Gamma(TC) \times \Gamma(TC) \rightarrow \mathcal{T}_1^1(\mathcal{C})$ is given by

$$\mathbf{R}(\tau_1, \tau_2) \tau_3 := \nabla_{\tau_1} \nabla_{\tau_2} \tau_3 - \nabla_{\tau_2} \nabla_{\tau_1} \tau_3 - \nabla_{[\tau_1, \tau_2]} \tau_3.$$

iii) \mathbf{Ric} and κ are defined analogously with $\bar{\mathbf{Ric}}$ and $\bar{\kappa}$ from the preceding definition.

Now we turn to the basic objects related to the embedding of a submanifold of arbitrary codimension.

Definition 8 Let $\tau, \tau_1, \tau_2 \in \Gamma(T\mathcal{C}), \nu \in \Gamma(N\mathcal{C})$.

i) The Weingarten mapping $\mathcal{W} : \Gamma(N\mathcal{C}) \rightarrow \mathcal{T}_1^1(\mathcal{C})$ is given by

$$\mathcal{W}(\nu)\tau := -P_T \bar{\nabla}_\tau \nu.$$

ii) The second fundamental form $\Pi(\cdot) : \Gamma(N\mathcal{C}) \rightarrow \times \mathcal{T}_2^0(\mathcal{C})$ is defined by

$$\Pi(\nu)(\tau_1, \tau_2) := \bar{g}(\bar{\nabla}_{\tau_1} \tau_2, \nu).$$

iii) The mean curvature normal $\eta \in \Gamma(N\mathcal{C})$ is defined to be the unique vector field that satisfies

$$\bar{g}(\eta, \nu) = \text{tr}_{\mathcal{C}} \mathcal{W}(\nu) \quad \forall \nu \in \Gamma(N\mathcal{C}).$$

iv) We define ∇^\perp to be the induced bundle connection on the normal bundle given via

$$\nabla_\tau^\perp \nu := P_\perp \bar{\nabla}_\tau \nu,$$

where ν and τ are canonically lifted to $T\mathcal{A} = T\mathcal{C} \times N\mathcal{C}$.

v) $R^\perp : \Gamma(T\mathcal{C}) \times \Gamma(T\mathcal{C}) \times \Gamma(N\mathcal{C}) \rightarrow \Gamma(N\mathcal{C})$ denotes the normal curvature mapping defined by

$$R^\perp(\tau_1, \tau_2)\nu := \nabla_{\tau_1}^\perp \nabla_{\tau_2}^\perp \nu - \nabla_{\tau_2}^\perp \nabla_{\tau_1}^\perp \nu - \nabla_{[\tau_1, \tau_2]}^\perp \nu.$$

Remark 4 i) The usual relations and symmetry properties for \mathcal{W} and Π also hold for codimension greater than one:

$$\Pi(\nu)(\tau_1, \tau_2) = g(\tau_1, \mathcal{W}(\nu)\tau_2) = g(\tau_2, \mathcal{W}(\nu)\tau_1) = \Pi(\nu)(\tau_2, \tau_1).$$

ii) A direct consequence of the definitions is the Weingarten equation:

$$\nabla_\tau^\perp \nu = \bar{\nabla}_\tau \nu + \mathcal{W}(\nu)\tau. \quad (97)$$

iii) The normal curvature mapping R^\perp is identically zero, when the dimension or the codimension of \mathcal{C} is smaller than two.

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