Effective Schrödinger Equations
on Submanifolds

vorgelegt von

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Zusammenfassung in deutscher Sprache

Die lineare Schrödingergleichung auf einem Konfigurationsraum $\mathcal{A}$ ist von der Form

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

wobei Δ der Laplace-Operator auf $\mathcal{A}$ und $V : \mathcal{A} \to \mathbb{R}$ das so genannte Potential ist. Obwohl ihre mathematische Struktur nicht besonders komplex ist, macht die hohe Dimension von $\mathcal{A}$ in vielen Fällen selbst eine numerische Lösung unmöglich. Daher ist es von großer Wichtigkeit, Situationen zu identifizieren, in denen die Dimension durch Approximation der Lösungen der ursprünglichen Gleichung (1) auf dem hochdimensionalen $\mathcal{A}$ durch Lösungen einer *effektiven Gleichung*

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

auf einem niederdimensionalen Konfigurationsraum $\mathcal{C}$ reduziert werden kann.

Ein sehr bedeutendes Beispiel dafür ist die zeitabhängige Born-Oppenheimer-Approximation: Die Schrödingergleichung für die Elektronen und Kerne eines Atoms,

$$\mathrm{i}\partial_t \psi \;=\; -\tfrac{1}{m_{\mathrm{nu}}}\Delta_x\,\psi \,-\, \tfrac{1}{m_{\mathrm{el}}}\Delta_y\,\psi \,+\, V_{\mathrm{ia}}\,\psi\,, \qquad \psi|_{t=0} \in L^2(\mathbb{R}^{d+k}, dx\,dy), \tag{2}$$

kann wegen der im Verhältnis zur Kernmasse m_{nu} sehr kleinen Elektronmasse m_{el} durch eine Gleichung approximiert werden, die nur noch die Kerne beschribt,

$$\mathrm{i}\partial_t \phi \;=\; -\tfrac{1}{m_{\mathrm{nu}}}\Delta_x\,\phi \,+\, E_{\mathrm{el}}\,\phi\,, \qquad \phi|_{t=0} \in L^2(\mathbb{R}^d, dx),$$

wobei die Wechselwirkungen aller Teilchen $V_{\mathrm{ia}}(x,y)$ durch die elektronischen Energieflächen $E_{\mathrm{el}}(x)$ ersetzt werden. Denn die leichten und daher schnellen Elektronen passen sich der Bewegung der schwereren und langsameren Kerne unmittelbar an in dem Sinne, dass der Zustand der Elektronen auf Grund der Skalenseparation bei den Massen stets bis auf kleine Fehler im von der Position der Kerne abhängigen Eigenzustand zur Energie E_{el} verbleibt und somit die Dynamik der Elektronen fast von der Dynamik der Kerne entkoppelt. Dies ist ein Spezialfall der so genannten *adiabatischen Entkopplung*, die typischerweise das Herleiten einer effektiven Dynamik erlaubt.

Eine andere physikalische Situation, in der eine solche Reduktion möglich scheint, sind mechanische Systeme mit Zwangsbedingungen. In diesen Systemen zwingen starke Kräfte die Zustände, effektiv in der Nähe einer Untermannigfaltigkeit $\mathcal{C}$ des Konfigurationsraums $\mathcal{A}$ zu verbleiben. Hier stellt

sich die naheliegende Frage, ob das System durch die Einschränkung von (1) auf $\mathcal{C}$,

$$\mathrm{i}\partial_t \phi \;=\; -\Delta_\mathcal{C}\,\phi \,+\, V|_\mathcal{C}\,\phi\,, \qquad \phi|_{t=0} \in L^2(\mathcal{C}, d\mu),$$

ersetzt werden kann, wobei $\Delta_\mathcal{C}$ der Laplace-Beltrami-Operator auf $\mathcal{C}$ ist. Dies wollen wir in der vorliegenden Arbeit möglichst genau und allgemein zugleich untersuchen. Es wird sich herausstellen, dass dies im Allgemeinen nicht der Fall ist, sondern sich eine effektive Gleichung ganz ähnlich zu der in der zeitabhängigen Born-Oppenheimer-Approximation ergibt.

An dieser Stelle führen wir das Modell, das wir betrachten, nur skizzenhaft ein und erläutern in erster Linie dessen Skalierung. Sei $(\mathcal{A}, G)$ eine Riemannsche Mannigfaltigkeit der Dimension $d + k$ und $\mathcal{C} \subset \mathcal{A}$ eine glatte Untermannigfaltigkeit der Dimension d ohne Rand und ausgestattet mit der induzierten Metrik $g = G|_\mathcal{C}$. Wir betrachten die Schrödingergleichung auf $\mathcal{A}$ mit einem Potential $V^\varepsilon : \mathcal{A} \to \mathbb{R}$, das für kleine ε eine gewisse Klasse von Zuständen in der Nähe von $\mathcal{C}$ lokalisiert.

Wir wollen also fest vorgegebene Mannigfaltigkeiten $\mathcal{A}$ und $\mathcal{C}$ betrachten und annehmen, dass das Potential in den zu $\mathcal{C}$ normalen Richtungen schnell groß wird, während die Variation entlang $\mathcal{C}$ im Vergleich dazu klein ist. Wir präzisieren diese Annahmen zunächst von einem mikroskopischen Standpunkt aus, d.h. die kleinste Ortsskala sei für den Moment von der Ordnung 1. Dann wollen wir annehmen, dass

- *normale Ableitungen des Potentials* von der Ordnung $\mathcal{O}(1)$ sind,

- *tangentiale Ableitungen des Potentials* von der Ordnung $\mathcal{O}(\varepsilon)$ sind,

- *alle Ableitungen der Metrik G* von der Ordnung $\mathcal{O}(\varepsilon)$ sind,

- und die Lösungen *Oszillationen* der Ordnung $\mathcal{O}(1)$ haben.

Oszillationen der Ordnung $\mathcal{O}(1)$ in normaler Richtung sind wichtig, um überhaupt Zustände zu finden, die in normaler Richtung lokalisiert sind. Dann erzeugt die Dynamik jedoch typischerweise auch Oszillationen der Ordnung $\mathcal{O}(1)$ in tangentialer Richtung.

Führen wir in der Umgebung eines Punkts $q \in \mathcal{C}$ lokale Koordinaten y auf $\mathcal{C}$ und n für die normalen Richtungen ein, so entsprechen obige Annahmen der Schrödingergleichung

$$\mathrm{i}\,\partial_t \Psi \;=\; -\Delta_{G^\varepsilon}\Psi \,+\, V(\varepsilon y, n)\Psi,$$

wobei G^ε die langsam variierende Metrik ist, die man durch Aufblasen von G erhält, und Δ_{G^ε} der zugehörige Laplace-Beltrami-Operator auf $\mathcal{A}$. Wechseln

wir nun durch Reskalieren der Koordinaten zu $(x = \varepsilon y, N = \varepsilon n)$ zurück zum makroskopischen Standpunkt, auf dem die Mannigfaltigkeiten nicht von ε abhängen, dann ergibt sich

$$i\,\partial_t \Psi^\varepsilon \;=\; -\varepsilon^2 \Delta_G \Psi^\varepsilon + V(x, N/\varepsilon)\Psi^\varepsilon, \tag{3}$$

weil der Laplace-Operator ein Differentialoperator zweiter Ordnung ist. Hier soll der obere Index ε an Ψ andeuten, dass wir an Lösungen interessiert sind, die Oszillationen der Ordnung $\mathcal{O}(\varepsilon^{-1})$ haben.

Für $\varepsilon \ll 1$ konzerntrieren sich die Lösungen dieser Gleichung bei der Untermannigfaltigkeit $\mathcal{C}$. Daher ist zu vermuten, dass eine effektive Schrödingergleichung auf $\mathcal{C}$ hergeleitet werden kann, so dass Lösungen $\psi_\varepsilon(t)$ der effektiven Gleichung die Lösungen $\Psi^\varepsilon(t)$ der vollen Gleichung in geeigneter Weise approximieren.

Die oben beschriebene Skalierung des Potentials war von der Wahl der Koordinaten abhängig und ist so nicht global durchführbar. Sie diente lediglich der Motivation. Um einen entsprechenden Skalierungslimes global implementieren zu können, nehmen wir an, dass die Untermannigfaltigkeit $\mathcal{C}$ eine offene Tubenumgebung $\mathcal{B}$ ohne Selbstdurchdringungen von festem Durchmesser $\delta > 0$ besitzt. Hier lässt sich sinnvoll postulieren, dass V^ε schnell bezüglich des Abstands zu $\mathcal{C}$ variiert. Da sich $\mathcal{B}$ isometrisch auf die δ-Umgebung $\mathcal{B}_\delta$ des Nullschnitts im Normalenbündel von $N\mathcal{C}$ abbilden lässt, kann diese Annahme auf Grund der dortigen linearen Struktur durch eine Skalierung des Potentials wie in (3) implementiert werden. Um später nur auf dem Normalenbündel arbeiten zu müssen, konstruieren wir einen Diffeomorphismus $\Phi : N\mathcal{C} \to \mathcal{B}$ und wählen eine Metrik $\overline{g}$ auf $N\mathcal{C}$, so dass Φ auf $\mathcal{B}_{\delta/2}$ eine Isometrie ist und für $\varepsilon \ll \delta$ die Lösungen unter einer beliebigen endlichen Energie bis auf Fehler kleiner als jede Potenz von ε in $\mathcal{B}_{\delta/2}$ liegen.

Um möglichst wenig Regularitätsprobleme zu haben, machen wir die folgenden technischen Annahmen.

Annahme 1: *Die Injektivitätsradien von $\mathcal{A}$ und $\mathcal{C}$ seien strikt positiv und alle Krümmungen sowie Ableitungen beliebiger Ordnung von diesen seien global beschränkt. Weiterhin sei $V : N\mathcal{C} \to \mathbb{R}$ glatt und beschränkt und beliebige Ableitungen von V seien ebenfalls beschränkt.*

Unser Ziel ist es nun, approximative Lösungen der Schrödingergleichung

$$i\,\partial_t \Psi^\varepsilon = -\varepsilon^2 \Delta_{\overline{g}} \Psi^\varepsilon + V(q, N/\varepsilon)\Psi^\varepsilon =: H^\varepsilon \Psi^\varepsilon$$

auf $\mathcal{H} = L^2(N\mathcal{C}, d\overline{\mu})$ zu finden, wobei $\overline{g}$ auf $\mathcal{B}_{\delta/2}$ der Rückzug von G mittels des Diffeomorphismus Φ und außerhalb von $\mathcal{B}_{\delta/2}$ geeignet fortgesetzt ist, sowie $d\overline{\mu}$ das zu $\overline{g}$ assozierte Maß bezeichnet.

Die grundlegende Idee dazu ist die folgende: Auf der Untermannigfaltigkeit $\mathcal{C}$ lässt sich der Laplace-Beltrami-Operator von $(N\mathcal{C}, \overline{g})$ wie folgt aufspalten:

$$\Delta_{\overline{g}} \,=\, \Delta_g \,+\, \Delta_N,$$

wobei Δ_g der Laplace-Beltrami-Operator auf $\mathcal{C}$ und Δ_N der Laplace-Operator in der Faser des Normalenbündels ist. Es zeigt sich, dass sich $\Delta_{\overline{g}}$, zumindest bis auf Fehler der Ordnung ε, global in Δ_N und einen geeigneten horizontalen Laplace-Operator Δ_{h} aufspalten lässt. Dann liefert das Reskalieren der normalen Koordinaten zu $n = N/\varepsilon$, dass

$$H_\varepsilon \,=\, -\varepsilon^2 \Delta_{\mathrm{h}} \,-\, \Delta_n \,+\, V(q,n) \,+\, \mathcal{O}(\varepsilon)\,. \tag{4}$$

Die Form dieses Operators ist dieselbe wie die des Hamilton-Operators (2), der der Ausgangspunkt für die Born-Oppenheimer-Approximation ist, wo ε der inversen Kernmasse entspricht. Dies legt nahe, dass auch in der hier betrachteten Situation adiabatische Entkopplung auftritt und sich somit die Methoden der adiabatischen Störungstheorie anwenden lassen.

Um die obige Aufspaltung zu erreichen, ist es hilfreich, das Maß auf $N\mathcal{C}$ in Produktform zu bringen. Dazu definieren wir

$$M_\rho : L^2(N\mathcal{C}, d\overline{\mu}) \to L^2(N\mathcal{C}, d\mu \otimes dN)\,, \quad \psi \mapsto M_\rho \psi := \sqrt{\rho}\, \psi\,,$$

wobei dN das Lebesgue-Maß auf $N_q\mathcal{C} \cong \mathbb{R}^k$ und $\rho = \frac{d\overline{\mu}}{d\mu \otimes dN}$ die Dichte des ursprünglichen Maßes und des Produktmaßes auf $N\mathcal{C}$ ist. M_ρ ist unitär und es gilt

$$M_\rho^* \left(-\Delta_{\overline{g}} \right) M_\rho \,=\, -\Delta_{\mathrm{h}} \,-\, \Delta_N \,+\, V_{\mathrm{geom}}(x) \,+\, \mathcal{O}(|N|)\,.$$

Die Transformation führt zum Auftauchen des rein geometrischen Extrapotentials V_{geom}. Daher ist der reskalierte Hamilton-Operator H_ε nach der unitären Transformation M_ρ in der Nähe von $\mathcal{C}$ von folgender Form :

$$H_\varepsilon \,=\, -\varepsilon^2 \Delta_{\mathrm{h}} \,-\, \Delta_n \,+\, V(x,n) \,+\, \varepsilon^2\, V_{\mathrm{geom}}(x) \,+\, \mathcal{O}(\varepsilon|n|)\,.$$

Man beachte, dass $-\varepsilon^2 \Delta_{\mathrm{h}}$ auf Funktionen mit Oszillationen der Ordnung ε^{-1} von der Ordnung 1 ist. Das Extrapotential spielt also zu führender Ordnung keine Rolle. Der verbleibende Fehlerterm ist allerdings nur dann wirklich klein, wenn er auf schnell abfallende Funktionen angewendet wird.

Wir erklären das Prinzip des adiabatischen Entkoppelns nun genauer. Dazu definieren wir für jedes $q \in \mathcal{C}$ den Faser-Hamilton-Operator auf dem Sobolev-Raum $W^{2,2}(N_q\mathcal{C}, dn) \subset L^2(N_q\mathcal{C}, dn)$ durch

$$H_{\mathrm{f}}(q) \,=\, -\Delta_n \,+\, V(q,\cdot)$$

und betrachten eine zugehörige q-abhängige Familie normalisierter Eigenfunktionen $\varphi_{\mathrm{f}}(q)$:

$$H_{\mathrm{f}}(q)\,\varphi_{\mathrm{f}}(q,\cdot) \;=\; E_{\mathrm{f}}(q)\,\varphi_{\mathrm{f}}(q,\cdot)\,. \tag{5}$$

Mittels (4) und (5) ist leicht zu sehen, dass Zustände aus dem Unterraum

$$\mathcal{P}_0 \;:=\; \{\psi(q)\varphi_{\mathrm{f}}(q,n) : \psi \in L^2(\mathcal{C},g)\} \subset L^2(N\mathcal{C})$$

näherungsweise invariant unter der Dynamik $\mathrm{e}^{-\mathrm{i}tH_\varepsilon}$ sind in dem Sinn, dass die Lösung der Schrödingergleichung zu Anfangsdaten $\Psi^\varepsilon|_{t=0} = \psi^\varepsilon\,\varphi_{\mathrm{f}}$ erfüllt, dass

$$\Psi^\varepsilon(t,q) \;=\; \psi^\varepsilon(t,q)\varphi_{\mathrm{f}}(q,n) + \mathcal{O}(\varepsilon|t|)\,,$$

wobei $\psi_\varepsilon(t,q)$ die folgende effektive Schrödingergleichung auf $\mathcal{C}$ löst:

$$\mathrm{i}\,\partial_t\psi^\varepsilon(t,q) \;=\; -\varepsilon^2\Delta_g\psi^\varepsilon(t,q) \;+\; E_{\mathrm{f}}(q)\,\psi^\varepsilon(t,q). \tag{6}$$

Eine Gleichung der Form (6) zeigt zwar erst auf der Zeitskala $s = t/\varepsilon$ ein interessantes Verhalten. Das adiabatische Prinzip besagt jedoch, dass $\mathcal{P}_0$ auch für solche und noch wesentlich längere Zeiten näherungsweise invariant ist, falls das Eigenwertband $(E_{\mathrm{f}})_q$ vom Rest des Spektrums geeignet separiert ist. Daher nehmen wir Folgendes an:

Annahme 2: *$H_{\mathrm{f}}(q)$ habe für alle $q \in \mathcal{C}$ einen einfachen Eigenwert $E_{\mathrm{f}}(q)$ mit*

$$\inf_{q\in\mathcal{C}}\mathrm{dist}\big(E_{\mathrm{f}}(q),\,\mathrm{Spektrum}(H_{\mathrm{f}}(q))\setminus E_{\mathrm{f}}(q)\,\big) \geq c_{\mathrm{gap}} > 0\,.$$

Die Einfachheit des Eigenwerts ist wichtig für uns, da sie in unserem Fall die Trivialisierbarkeit des zugehörigen Eigenraumbündels impliziert, also die Existenz einer global glatten Familie normalisierter Eigenfunktionen $\varphi_{\mathrm{f}}(q)$ sicherstellt. Da die Aufspaltung $\Delta_{\overline{g}} = \Delta_{\mathrm{h}} + \Delta_N + \mathcal{O}(\varepsilon)$ wie oben erläutert nur in der Nähe von $\mathcal{C}$ gültig war, brauchen wir außerdem, dass φ_{f} exponentiell abfällt, was jedoch in sehr vielen Fällen durch Annahme 2 impliziert wird. Die Annahmen 1 und 2 sowie exponentiellen Abfall von φ_{f} in normalen Richtungen vorausgesetzt, lässt sich das folgende Resultat beweisen.

Theorem: *Fixiere $E_{\max} < \infty$. Unter den obigen Annahmen gibt es eine Riemannsche Metrik $g_{\mathrm{eff}}^\varepsilon$ auf $\mathcal{C}$ mit assoziiertem Maß $d\mu_{\mathrm{eff}}^\varepsilon$, einen selbstadjungierten Operator $H_{\mathrm{eff}}^\varepsilon$ auf $L^2(\mathcal{C}, d\mu_{\mathrm{eff}}^\varepsilon)$, $C < \infty$ und $\varepsilon_0 > 0$, so dass für den Operator $U_0 : \mathcal{P}_0 \to L^2(\mathcal{C}, d\mu_{\mathrm{eff}}^\varepsilon)$ definiert durch*

$$U_0^* : L^2(\mathcal{C}, d\mu_{\mathrm{eff}}^\varepsilon) \to \mathcal{H}\,, \quad \psi^\varepsilon(q) \mapsto \psi^\varepsilon(q)\,\varphi_{\mathrm{f}}(q,n)$$

sowie alle $\varepsilon < \varepsilon_0$ und Borelfunktionen χ mit $\mathrm{supp}\,\chi \subset (-\infty, E_{\max}]$ gilt, dass

$$\big\|\big(\mathrm{e}^{-\mathrm{i}H_\varepsilon t} - U_0^*\,\mathrm{e}^{-\mathrm{i}H_{\mathrm{eff}}^\varepsilon t}\,U_0\big)\,U_0^*\,\chi(H_{\mathrm{eff}}^\varepsilon)\,U_0\big\|_{\mathcal{L}(\mathcal{H})} \;<\; C\,\varepsilon\,(1 + \varepsilon|t|)\,. \tag{7}$$

Hier ist $\chi(H_{\mathrm{eff}}^{\varepsilon})$ durch den Spektralsatz definiert. Der effektive Hamilton-Operator ist beschrieben durch:

$$\langle \psi,\, H_{\mathrm{eff}}^{\varepsilon}\, \psi \rangle \;=\; \int_{\mathcal{C}} g_{\mathrm{eff}}^{\varepsilon} \big(\overline{p_{\mathrm{eff}}^{\varepsilon}\, \psi},\, p_{\mathrm{eff}}^{\varepsilon}\, \psi \big) \,+\, E_{\mathrm{f}} |\psi|^2 \; d\mu_{\mathrm{eff}}^{\varepsilon}$$

mit $p_{\mathrm{eff}}^{\varepsilon} \,=\, -\mathrm{i}\varepsilon\mathrm{d} + \varepsilon \,\langle \varphi_{\mathrm{f}}, \mathrm{i}\nabla^{\mathrm{h}}\varphi_{\mathrm{f}}\rangle$ und $g_{\mathrm{eff}}^{\varepsilon} \,=\, g + \varepsilon \,\mathrm{II}_{\alpha}(\langle \varphi_{\mathrm{f}}, n^{\alpha}\varphi_{\mathrm{f}}\rangle)$, wobei ∇^{h} eine geeignete horizontale Ableitung und II_{α} die zweite Fundamentalform zur Richtung n^{α} ist.

Mittels des Operators U_0^{*} lassen sich also aus den Lösungen der effektiven Gleichung approximative Lösungen der vollen Gleichung gewinnen. Man beachte, dass $U_0^{*}\chi(H_{\mathrm{eff}}^{\varepsilon})U_0$ sowohl hohe Energien abschneidet als auch dafür sorgt, dass die Anfangsdaten in $\mathcal{P}_0$ liegen. Das Abschneiden der Energien durch χ erfolgt unabhängig von ε und erlaubt somit, dass $\langle \psi| -\varepsilon^2\Delta_g\psi\rangle$ von der Ordnung $\mathcal{O}(1)$ ist, also Oszillationen auf der Skala ε^{-1} auftreten. Aus dem obigen Resultat lässt sich auch folgern, dass die unteren Bereiche der Spektren von H_{ε} und $H_{\mathrm{eff}}^{\varepsilon}$ nahe beieinander liegen.

Für Zeiten der Ordnung $\mathcal{O}(\varepsilon^{-1})$ liefern die Korrekturen zum Impuls $p_{\mathrm{eff}}^{\varepsilon}$ und zur Metrik $g_{\mathrm{eff}}^{\varepsilon}$ relevante Beiträge. Hier ist anzumerken, dass $\mathrm{i}p_{\mathrm{eff}}^{\varepsilon}$ ein Zusammenhang auf dem komplexen Linienbündel über $\mathcal{C}$ ist, wo die effektive Wellenfunktion ihre Werte annimmt. Dieser so genannte Berry-Zusammenhang ist zwar stets flach, kann jedoch über eine nicht-triviale Holonomie verfügen.

Wenn der Eigenwert E_{f} konstant auf ganz $\mathcal{C}$ ist, wird es interessant, auch Zeiten der Ordnung $\mathcal{O}(\varepsilon^{-2})$ zu betrachten. Daher werden wir im Hauptteil dieser Arbeit ein wesentlich allgemeineres Resultat, das auch für solche Zeiten noch kleine Fehler liefert, beweisen. Um dies zu erreichen, konstruieren wir mittels adiabatischer Störungstheorie einen Projektor P_{ε}, der zu führender Ordnung auf $\mathcal{P}_0$ projeziert, so dass der Kommutator $[H_{\varepsilon}, P_{\varepsilon}]$ von der Ordnung $\mathcal{O}(\varepsilon^3)$ ist. Dann lässt sich relativ leicht zeigen, dass die Fehler in (7) nur noch von der Größe $\varepsilon\,(1+\varepsilon^2|t|)$ sind, wenn man im zu P_{ε} gehörigen Unterraum startet und in $H_{\mathrm{eff}}^{\varepsilon}$ Terme der Ordnung $\mathcal{O}(\varepsilon^2)$ ergänzt.

Formal funktioniert die Konstruktion von P_{ε} wie folgt: Nach Definition von H_{f} gilt für schnell abfallende Funktionen, dass $H_{\varepsilon} \,=\, H_{\mathrm{f}} - \varepsilon^2\Delta_{\mathrm{h}} + \mathcal{O}(\varepsilon)$. Wie schon erläutert wurde, ist $\mathcal{P}_0$ näherungsweise invariant unter der zu H_{ε} gehörenden Dynamik. Dies liegt daran, dass der zugehörige Projektor P_0 definiert durch $(P_0\Psi)(q,n) := \varphi_{\mathrm{f}}(q,n)\,\langle \varphi_{\mathrm{f}}|\Psi\rangle(q)$ offensichtlich mit H_{f} kommutiert und somit

$$[H_{\varepsilon}, P_0] \;=\; [-\varepsilon^2\Delta_{\mathrm{h}}, P_0] + \mathcal{O}(\varepsilon) \;=\; \mathcal{O}(\varepsilon) \;=:\; \varepsilon A + \mathcal{O}(\varepsilon^2).$$

Wegen $P_0^2 = P_0$ verschwindet der diagonale Anteil von A bezüglich P_0, d.h.

$$A \;=\; P_0\, A\,(1 - P_0) + (1 - P_0)\, A\, P_0.$$

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Diese Einsichten legen den Ansatz $P_\varepsilon = P_0 + \varepsilon P_1 + \varepsilon^2 P_2 + \varepsilon^3 P_3$ nahe. Nun wollen wir P_1 so wählen, dass

$$[H_\varepsilon, P_\varepsilon] = \varepsilon A + \varepsilon[H_\varepsilon, P_1] + \mathcal{O}(\varepsilon^2) \overset{!}{=} \mathcal{O}(\varepsilon^2).$$

Wir setzen $P_1 := T^* P_0 + P_0 T$ mit noch zu bestimmendem T und nehmen zunächst an, dass $[T, -\varepsilon^2 \Delta_\mathrm{h} + E_\mathrm{f}] = \mathcal{O}(\varepsilon)$ gilt. Damit ist

$$
\begin{aligned}
[H_\varepsilon, P_1] &= [H_\mathrm{f} - \varepsilon^2 \Delta_\mathrm{h}, T^* P_0 + P_0 T] + \mathcal{O}(\varepsilon) \\
&= [H_\mathrm{f} - E_\mathrm{f}, T^* P_0] + [H_\mathrm{f} - E_\mathrm{f}, P_0 T] + O(\varepsilon) \\
&= (H_\mathrm{f} - E_\mathrm{f})(1 - P_0) T^* P_0 - P_0 T (1 - P_0)(H_\mathrm{f} - E_\mathrm{f}) + \mathcal{O}(\varepsilon),
\end{aligned}
$$

wobei wir im letzten Schritt benutzt haben, dass $(H_\mathrm{f} - E_\mathrm{f})P_0 = 0$ ist. Da $H_\mathrm{f} - E_\mathrm{f}$ wegen Annahme 2 auf dem Bild von $1 - P_0$ stetig invertierbar ist, erhalten wir

$$
\begin{aligned}
(1 - P_0) T^* P_0 &= (H_\mathrm{f} - E_\mathrm{f})^{-1} (1 - P_0) A P_0, \\
P_0 T (1 - P_0) &= -P_0 A (1 - P_0) (H_\mathrm{f} - E_\mathrm{f})^{-1}.
\end{aligned}
$$

Dies legt T jenseits der Diagonalen fest. Um am Schluss tatsächlich einen Projektor aus P_ε machen zu können, wählt man den diagonalen Anteil so, dass $(P_0 + \varepsilon P_1)^2 = P_0 + \varepsilon P_1 + \mathcal{O}(\varepsilon^2)$ gilt. Es stellt sich heraus, dass die oben gemachte Annahme $[T, -\varepsilon^2 \Delta_\mathrm{h} + E_\mathrm{f}] = \mathcal{O}(\varepsilon)$ bei dieser Wahl von T automatisch erfüllt ist. Analog zum Vorgehen bei P_1 bestimmt man auch die verschiedenen Anteile von P_2. Durch geschickte Wahl von P_3 erhält man dann einen Projektor.

Die Konstruktion von P_ε ist jedoch mit einigen größeren technischen Hürden verbunden. So ist einerseits schon der Kommutator $[H_\varepsilon, P_0]$ und damit auch unser formales T ein unbeschränkter Operator, was es erforderlich macht, zwischendurch immer wieder die hohen Energien abzuschneiden. Andererseits müssen wir sicherstellen, dass aus dem Abfall von φ_f auch ein genügend schneller Abfäll des Bildes von P_ε folgt, so dass man wirklich alle Objekte durch ihre Approximation in der Nähe von $\mathcal{C}$ ersetzen kann.

Dieser kurze Überblick über die Ideen, die dieser Arbeit zu Grunde liegen, enthält keine Informationen, die nicht auch in einem der späteren Kapitel zu finden sind. Er sollte jedoch für das Verständnis des Vorgehens hilfreich sein.

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1 Introduction

Although the mathematical structure of the linear Schrödinger equation

$$i\partial_t \psi = -\Delta\psi + V\psi =: H\psi\,, \qquad \psi|_{t=0} \in L^2(\mathcal{A}, d\tau) \qquad (8)$$

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 (8) on the high dimensional configuration space $\mathcal{A}$ by solutions of an *effective equation*

$$i\partial_t \phi = H_{\text{eff}}\phi\,, \qquad \phi|_{t=0} \in L^2(\mathcal{C}, d\mu) \qquad (9)$$

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

The physically most straight forward 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 [11] 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 (9) of the form

$$H_{\text{eff}} = -\Delta_{\mathcal{C}} + V|_{\mathcal{C}}\,, \qquad (10)$$

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 $V : \mathcal{A} \to \mathbb{R}$ to $\mathcal{C}$.

However, to justify or invalidate the above procedures from first principles, one needs to model the constraining forces within the dynamics (8) 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 (8) in the asymptotic limit where the constraining forces become very strong and tries to extract a 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 and Ungar [38], 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 of older results, as well as the book of Hairer, Lubich and Wanner [17], Section XIV.3, for an approach based on classical adiabatic invariants.

For the quantum mechanical case Marcus [27] and later on Jensen and Koppe [21] 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 [8] 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 (10), i.e. a Hamiltonian that depends only on the intrinsic geometry of $\mathcal{C}$ and the restriciton 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 of (8). In this work we present and prove a general result concerning the precise form of the limiting dynamics (9) on $\mathcal{C}$ starting from (8) 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 [15], Maraner [25] and Mitchell [30], 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 with the methods used in [8, 25, 15, 30] only for solutions with bounded kinetic energies in the tangential directions. Therefore the transfer of energy between normal and tangential modes was excluded in those articles 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 [30].

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-Sordoni and Panati-Spohn-Teufel in [28, 29, 32, 34, 41, 43], 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 [6], 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: Teufel solved the problem for constraint manifolds $\mathcal{C}$ which are d-dimensional subspaces of $\mathbb{R}^{d+k}$ in [43] , while Dell'Antonio and Tenuta [10] considered the leading order behavior of semiclassical Gaussian wave packets for general geometries.

Another result about submanifolds of any dimension is due to Wittich [44], 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 [16] 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 non-technical sketch of the structure of our result. The detailed statements given in 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 non-trivial 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 [15, 30], 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

$$\mathrm{i}\partial_t \psi^\varepsilon \;=\; -\varepsilon^2 \Delta_{NC}\psi^\varepsilon \;+\; V_{\mathrm{c}}(q,\varepsilon^{-1}\nu)\psi^\varepsilon \;+\; W(q,\nu)\psi^\varepsilon \;=:\; H^\varepsilon \psi^\varepsilon \quad (11)$$

for $\psi^\varepsilon|_{t=0} \in L^2(NC)$. Here Δ_{NC} is the Laplace-Beltrami operator on NC, where the metric on NC is obtained by pulling back the metric on a tubular neighborhood of C in A to a tubular neighborhood of the zero section in NC and then suitably extending it to all of NC. We study the asymptotic behavior of (11) 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 $\|\varepsilon\nabla^{\mathrm{h}}\psi_0^\varepsilon\|^2 = \langle \psi_0^\varepsilon \,|\, -\varepsilon^2\Delta_{\mathrm{h}}\psi_0^\varepsilon\rangle$ is of order one, in contrast to the earlier works [15, 30], 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 (9). It is presented in two steps. In Section 2.1 it is stated that on certain subspaces of $L^2(NC)$ the unitary group $\exp(-\mathrm{i}H^\varepsilon t)$ generating solutions of (11) is unitarily equivalent to an 'effective' unitary group $\exp(-\mathrm{i}H_{\mathrm{eff}}^\varepsilon t)$ associated to (9) up to errors of order $\varepsilon^3|t|$ uniformly for bounded initial energies. In Section 2.2 we provide the asymptotic expansion of $H_{\mathrm{eff}}^\varepsilon$ up to terms of order ε^2, i.e. we compute $H_{\mathrm{eff},0}$, $H_{\mathrm{eff},1}$ and $H_{\mathrm{eff},2}$ in $H_{\mathrm{eff}} = H_{\mathrm{eff},0} + \varepsilon H_{\mathrm{eff},1} + \varepsilon^2 H_{\mathrm{eff},2} + \mathcal{O}(\varepsilon^3)$. Furthermore, in Section 2.3 and 2.4 we explain how to obtain quasimodes of H^ε from the eigenfunctions of $H_{\mathrm{eff},0} + \varepsilon H_{\mathrm{eff},1} + \varepsilon^2 H_{\mathrm{eff},2}$ and quasimodes of $H_{\mathrm{eff},0} + \varepsilon H_{\mathrm{eff},1} + \varepsilon^2 H_{\mathrm{eff},2}$ from the eigenfunctions of H^ε and apply our formulas to quantum wave guides, i.e. the special case of curves in $\mathbb{R}^3$. As corollaries we obtain results generalizing in some respects those by Friedlander and Solomyak obtained in [14] and by Bouchitté et al. in [5]. In addition, we discuss how twisted closed wave guides display phase shifts somewhat similar to the Aharanov-Bohm effect but without magnetic fields!

The crucial step in the proof is the construction of closed infinite dimensional subspaces of $L^2(NC)$ which are invariant under the dynamics (11) up to small errors and which can be mapped unitarily to $L^2(C)$, where the effective dynamics takes place. To construct these 'almost invariant subspaces', we define at each point $q \in C$ a Hamiltonian operator $H_{\mathrm{f}}(q)$ acting on the fibre $N_q C$. If it has a simple eigenvalue band $E_{\mathrm{f}}(q)$ that depends smoothly on q and is isolated from the rest of the spectrum for all q, then the corresponding eigenspaces define a smooth line bundle over C. Its L^2-sections define a closed subspace of $L^2(NC)$, which after a modification of order ε becomes the almost invariant subspace associated to the eigenvalue band $E_{\mathrm{f}}(q)$. In

the end, to each isolated eigenvalue band $E_f(q)$ there is an associated line bundle over $\mathcal{C}$, an associated almost invariant subspace and an associated effective Hamiltonian H_{eff}^ε.

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

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

We note that $(V_c + W)|_\mathcal{C}$ is contained in E_f. This is the quantum version of the result of Rubin and Ungar [38] for classical mechanics. However, the time scale for which the solutions of (11) propagate along finite distances are times t of order ε^{-1}. On this longer time scale the first order correction $\varepsilon H_{eff,1}$ to the effective Hamiltonian has effects of order one and must be included in the effective dynamics. We do not give the details of $H_{eff,1}$ 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 one to a non-trivial one, the so-called generalized Berry connection. For the normal eigenfunction may vary in shape along the submanifold which induces a non-trivial connection on the line bundle associated to the eigenvalue band $E_f(q)$. This was already discussed by Mitchell in the case that the potential (and thus the eigenfunctions) only twists.

When E_f is constant as in the earlier works, there is no non-trivial potential term up to first order and so the second order corrections in $H_{eff,2}$ become relevant. They 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 occurence had originally 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.

We 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 $H_{eff,2}$. That is why the extra potential depending on curvature appeared at leading order in these works, while it appears only in $H_{eff,2}$ for us. And this is also the reason that assumptions were necessary, assuring that all other terms appearing in our $H_{eff,0}$ and $H_{eff,1}$ are of higher order or trivial, including that $E_f(q) \equiv E_f$ 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 $E_f(q)$. With one caveat, it extends to degenerate eigenvalues in a straightforward way. Our construction requires the complex line bundle associated with $E_f(q)$ to be trivializable. For line bundles, triviality follows from the vanishing of the first Chern class. And for real Hamiltonians like H^ε in (11) it turns out that the complex line bundle associated to $E_f(q)$ always has vanishing first Chern class. However, for degenerate eigenvalue bands no such argument is available (except for a compact $\mathcal{C}$ with $\dim \mathcal{C} \le 3$, see Panati [33]) 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 $E_f(q)$.

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 neighborhood of $\mathcal{C}$ in $\mathcal{A}$ to the whole normal bundle, $N\mathcal{C}$ with this metric has curvature increasing linearly with the distance to $\mathcal{C}$. 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 12).

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/codimension k, which is equipped with the induced metric $g = G|_{\mathcal{C}}$ and the associated 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 $T\mathcal{A}|_{\mathcal{C}} = T\mathcal{C} \times N\mathcal{C}$ of $\mathcal{A}$'s tangent

bundle into the tangent and the normal bundle of $\mathcal{C}$. We assume that there exists a tubular neighborhood $\mathcal{B} \subset \mathcal{A}$ of $\mathcal{C}$ with globally fixed diameter, that is there is $\delta > 0$ such that normal geodesics γ (i.e. $\gamma(0) \in \mathcal{C}, \dot{\gamma}(0) \in N\mathcal{C}$) of length δ do not intersect. We will call a tubular neighborhood of radius r an r-tube. Furthermore, we assume that

$$\mathcal{A} \ and \ \mathcal{C} \ are \ of \ bounded \ geometry \qquad (12)$$

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

$$\mathcal{C} \hookrightarrow \mathcal{A} \ has \ globally \ bounded \ derivatives \ of \ any \ order, \qquad (13)$$

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

$$\mathrm{i}\partial_t \psi \ = \ -\Delta_{\mathcal{A}}\psi \ + \ V_{\mathcal{A}}^{\varepsilon}\psi, \qquad \psi|_{t=0} \in L^2(\mathcal{A}, d\tau), \qquad (14)$$

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 by ε^{-1} in the directions normal to the submanifold. We emphasize that we will not assume $V_{\mathcal{A}}^{\varepsilon}$ to become large away from $\mathcal{C}$, which makes the proof of localization more difficult.
In order to actually implement the scaling in the normal directions, we will now construct a related problem on the normal bundle of $\mathcal{C}$ by mapping $N\mathcal{C}$ diffeomorphically to the tubular neighborhood $\mathcal{B}$ of $\mathcal{C}$ in a specific way and then choosing a suitable metric $\overline{g}$ on $N\mathcal{C}$ (considered as a manifold). On the normal bundle the scaling of the potential in the normal directions is straight forward. 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 $\overline{g}$ and of the horizontal and vertical derivatives ∇^{h} and ∇^{v} and to immediately jump to the end of Definiton 1.

The mapping to the normal bundle is performed in the following way. There is a natural diffeomorphism from the δ-tube $\mathcal{B}$ to the δ-neighborhood $\mathcal{B}_{\delta}$ 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 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 $\tilde{\Phi} \in C^\infty\big(\mathbb{R}, (-\delta, \delta)\big)$ which is the identity on $(-\delta/2, \delta/2)$ and satisfies

$$\forall\, j \in \mathbb{N} \quad \exists\, C_j < \infty \quad \forall\, r \in \mathbb{R}: \quad |\tilde{\Phi}^{(j)}(r)| \;\leq\; C_j\,(1 + r^2)^{-(j+1)/2} \qquad (15)$$

(see Figure 1). Now a diffeomorphism $\Phi \in C^\infty(N\mathcal{C}, \mathcal{B})$ 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 charts in the normal directions.
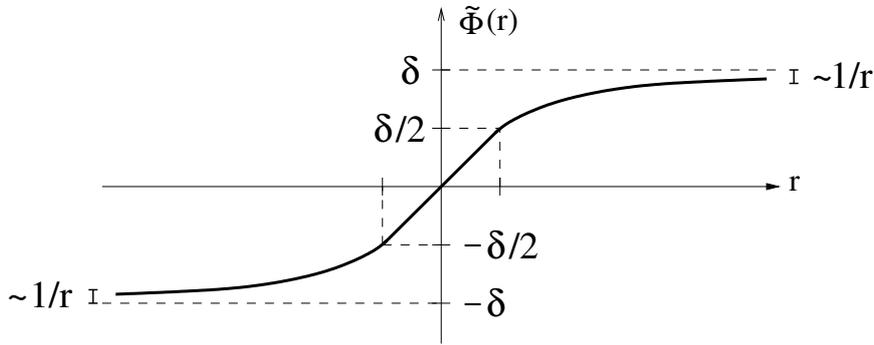

Figure 1: $\tilde{\Phi}$ converges to $\pm\delta$ like $1/r$.

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 $\Phi^* G$ of G on $\mathcal{B}_{\delta/2}$. 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 $N\mathcal{C} \setminus \mathcal{B}_\delta$ 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 $N\mathcal{C}$; 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 latter two properties globally is the so-called Sasaki metric which is defined in the following way (see e.g. Ch. 9.3 of [1]): The Levi-Civita connection on $\mathcal{A}$ induces a connection ∇ on $T\mathcal{C}$, which coincides with the Levi-Civita connection on $(\mathcal{C}, g)$, and a connection $\nabla^\perp$ on $N\mathcal{C}$, which is called the *normal connection* (see the appendix). The normal connection itself induces the connection map $K : TN\mathcal{C} \to N\mathcal{C}$ which identifies the vertical subspace of $T_{(q,\nu)}N\mathcal{C}$ with $N_q\mathcal{C}$. Let $\pi : N\mathcal{C} \to \mathcal{C}$ be the bundle projection. The Sasaki metric is then given by

$$g^{\mathrm{S}}_{(q,\nu)}(v, w) \;:=\; g_q(\mathrm{D}\pi\, v, \mathrm{D}\pi\, w) \,+\, G_{(q,0)}(Kv, Kw). \qquad (16)$$

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It was studied by Wittich in [44] in a similar context. The completeness of $(N\mathcal{C}, g^{\mathrm{S}})$ follows from the completeness of $\mathcal{C}$ (see the proof for $T\mathcal{C}$ by Liu in [24]). $\mathcal{C}$ is complete because it is of bounded geometry. But $(N\mathcal{C}, g^{\mathrm{S}})$ is, in general, not of bounded geometry, as it has curvatures growing polynomially in the fibers. However, $(\mathcal{B}_r \subset N\mathcal{C}, g^{\mathrm{S}})$ is a subset of bounded geometry for any $r < \infty$. 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

$$\overline{g}_{(q,\nu)}(v, w) \;:=\; \Theta(|\nu|)\, G_{\Phi(q,\nu)}(\mathrm{D}\Phi\, v, \mathrm{D}\Phi\, w) \;+\; \big(1 - \Theta(|\nu|)\big)\, g^{\mathrm{S}}_{(q,\nu)}(v, w) \quad (17)$$

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

$$|\nu| = \sqrt{\overline{g}_{(q,0)}(\nu, \nu)}. \qquad (18)$$

The Levi-Civita connection on $(N\mathcal{C}, \overline{g})$ will be denoted by $\overline{\nabla}$ and the volume measure associated to $\overline{g}$ by $d\overline{\mu}$. We note that $\mathcal{C}$ is still isometrically imbedded and that $\overline{g}$ induces the same bundle connections ∇ and $\nabla^{\perp}$ on $T\mathcal{C}$ and $N\mathcal{C}$ as G. Since $\mathcal{A}$ is of bounded geometry and $(\mathcal{B}_{\delta}, g^{\mathrm{S}})$ is a subset of bounded geometry, $(\mathcal{B}_{\delta}, \overline{g})$ is a subset of bounded geometry. Furthermore, $(N\mathcal{C}, \overline{g})$ is complete due to the metric completeness of $(\overline{\mathcal{B}}_{\delta}, \Phi^*G)$ (implied by the bounded geometry of $\mathcal{A}$) and the completeness of $(N\mathcal{C}, g^{\mathrm{S}})$.

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 [44]). Together with the bounded geometry of $(\mathcal{B}_{\delta}, \overline{g})$ and $(\mathcal{B}_{\delta}, g^{\mathrm{S}})$, which implies that all small enough balls with the same radius have comparable volume (see [40]), we obtain that

$$\frac{d\overline{\mu}}{d\mu \otimes d\nu}\Big|_{(N\mathcal{C} \setminus \mathcal{B}_{\delta/2}) \cup \mathcal{C}} \equiv 1, \quad \frac{d\overline{\mu}}{d\mu \otimes d\nu} \in C^{\infty}_{\mathrm{b}}(N\mathcal{C}), \quad \frac{d\overline{\mu}}{d\mu \otimes d\nu} \geq c > 0, \quad (19)$$

where $C^{\infty}_{\mathrm{b}}(N\mathcal{C})$ is the space of smooth functions on $N\mathcal{C}$ with all its derivatives globally bounded with respect to $\overline{g}$.

Since we will think of the functions on $N\mathcal{C}$ 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 hermitian bundle $\mathcal{E}$ and by $\Gamma_{\mathrm{b}}(\mathcal{E})$ the ones with globally bounded derivatives up to any order.*

i) Fix $q \in \mathcal{C}$. The fiber $(N_q\mathcal{C}, \overline{g}_{(q,0)})$ 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 $(q, \nu) \in N_q\mathcal{C}$.

Let $\varphi \in C^1(N_q\mathcal{C})$. The vertical derivative *$\nabla^{\mathrm{v}}\varphi \in N_q^*\mathcal{C}$ at $\nu \in N_q\mathcal{C}$ is the pullback via ι of the exterior derivative of $\varphi \in C^1(N_q\mathcal{C})$ to $N_q^*\mathcal{C}$. i.e.*

$$(\nabla^{\mathrm{v}}_\zeta \varphi)(\nu) \;=\; (\mathrm{d}\varphi)_\nu\big(\iota(\zeta)\big)$$

for $\zeta \in N_q\mathcal{C}$. The Laplacian associated to $-\int_{N_q\mathcal{C}} \overline{g}_{(q,0)}(\nabla^{\mathrm{v}}\varphi, \nabla^{\mathrm{v}}\varphi) d\nu$ is denoted by Δ_{v} and the set of bounded functions with bounded derivatives of arbitrary order by $C^\infty_{\mathrm{b}}(N_q\mathcal{C})$.

ii) Let $\mathcal{E}_{\mathrm{f}} := \{(q, \varphi) \,|\, q \in \mathcal{C}, \varphi \in C^\infty_{\mathrm{b}}(N_q\mathcal{C})\}$ be the bundle over $\mathcal{C}$ which is obtained by replacing the fibers $N_q\mathcal{C}$ of the normal bundle with $C^\infty_{\mathrm{b}}(N_q\mathcal{C})$ and canonically lifting the action of $\mathrm{SO}(k)$ and thus the bundle structure of $N\mathcal{C}$. The horizontal connection *∇^{h} on $\mathcal{E}_{\mathrm{f}}$ is defined by*

$$(\nabla^{\mathrm{h}}_\tau \varphi)(q, \nu) \;:=\; \frac{d}{ds}\Big|_{s=0} \varphi(w(s), v(s)), \tag{20}$$

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

$$w(0) \;=\; q, \;\; \dot{w}(0) \;=\; \tau(q), \quad \& \quad v(0) \;=\; \nu, \; \nabla^\perp_{\dot{w}} v \;=\; 0.$$

Furthermore, Δ_{h} is the Bochner Laplacian associated to ∇^{h}:

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

where we have used the same letter g for the canonical shift of g from the tangent bundle to the cotangent bundle of $\mathcal{C}$. Higher order horizontal derivatives are inductively defined by

$$\nabla^{\mathrm{h}}_{\tau_1, \ldots, \tau_m} \varphi \;:=\; \nabla^{\mathrm{h}}_{\tau_1} \nabla^{\mathrm{h}}_{\tau_2, \ldots, \tau_m} \varphi - \sum_{j=2}^{m} \nabla^{\mathrm{h}}_{\tau_2, \ldots, \nabla_{\tau_1}\tau_j, \ldots, \tau_m} \varphi$$

for arbitrary $\tau_1, \ldots, \tau_m \in \Gamma(T\mathcal{C})$. The set of bounded sections φ of $\mathcal{E}_{\mathrm{f}}$ such that $\nabla^{\mathrm{h}}_{\tau_1, \ldots, \tau_m} \varphi$ is also a bounded section for all $\tau_1, \ldots, \tau_m \in \Gamma_{\mathrm{b}}(T\mathcal{C})$ is denoted by $C^m_{\mathrm{b}}(\mathcal{C}, C^\infty_{\mathrm{b}}(N_q\mathcal{C}))$.

Coordinate expressions for ∇^{v} and ∇^{h} are calculated at the beginning of Section 4.

In the following, we consider the Hilbert space $\overline{\mathcal{H}} := L^2\big((N\mathcal{C}, \overline{g}), d\overline{\mu}\big)$ of complex-valued square-integrable functions. We emphasize that the elements of $\overline{\mathcal{H}}$ take values in the trivial complex line bundle over $N\mathcal{C}$. This will be the case for all functions throughout the whole text 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 $\langle\,.\,|\,.\,\rangle_{\mathcal{H}}$ and the induced norm by $\|\,.\,\|_{\mathcal{H}}$. The upper index $*$ will be used for both the adjoint of an operator and the complex conjugation of a function.

Instead of (14) we now consider a Schrödinger equation on the normal bundle, thought of as a Riemannian manifold $(N\mathcal{C}, \overline{g})$. There we can immediately implement the idea of squeezing the potential in the normal directions: Let

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

for fixed real-valued potentials $V_{\mathrm{c}}, W \in C_{\mathrm{b}}^\infty(\mathcal{C}, C_{\mathrm{b}}^\infty(N_q\mathcal{C}))$. 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.
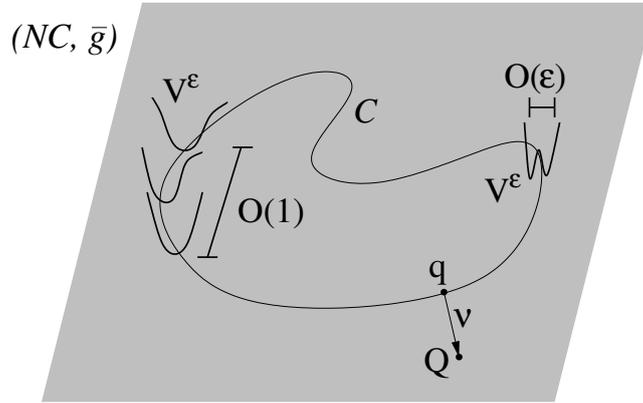
Figure 2: The width of V_ε is ε but it varies on a scale of order one along $\mathcal{C}$.

We will investigate the Schrödinger equation

$$\mathrm{i}\partial_t\psi = H^\varepsilon\psi := -\varepsilon^2\Delta_{N\mathcal{C}}\psi + V^\varepsilon\psi, \qquad \psi|_{t=0} = \psi_0^\varepsilon \in \overline{\mathcal{H}}, \qquad (21)$$

where $\Delta_{N\mathcal{C}}$ is the Laplace-Beltrami operator on $(N\mathcal{C}, \overline{g})$, i.e. the operator associated to $-\int_{N\mathcal{C}}\overline{g}(d\psi, d\psi)d\overline{\mu}$. To ensure proper scaling behavior, we need

to multiply the Laplacian in (21) 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 for ε-dependent initial data ψ_0^ε with tangential kinetic energy $\langle \psi_0^\varepsilon | -\varepsilon^2 \Delta_{\mathrm h} \psi_0^\varepsilon \rangle$ 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 $V_{\mathrm c}$ and W to be bounded. In Section 1.3 of [40] H^ε is shown to be selfadjoint on its maximal domain $\mathcal{D}(H^\varepsilon)$ for any complete Riemannian manifold $\mathcal{M}$, thus in particular for $(N\mathcal{C}, \overline{g})$. Let $W^{2,2}(N\mathcal{C}, \overline{g})$ be the second Sobolev space, i.e. the set of all L^2-functions with square-integrable covariant derivatives up to second order. We emphasize that, in general, $W^{2,2}(N\mathcal{C}, \overline{g}) \subset \mathcal{D}(H^\varepsilon)$ but $W^{2,2}(N\mathcal{C}, \overline{g}) \neq \mathcal{D}(H^\varepsilon)$ for a manifold of unbounded geometry.

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 $\rho := \frac{d\overline{\mu}}{d\mu \otimes d\nu}$ of our starting measure and the product measure on $N\mathcal{C}$ that was introduced above. We recall from (19) that this density is bounded and strictly positive. After the transformation it is helpful to rescale the normal directions.

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

i) The unitary transform M_ρ is defined by $M_\rho : \mathcal{H} \to \overline{\mathcal{H}}, \ \psi \mapsto \rho^{\frac{1}{2}}\psi$.

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*

$$ H_\varepsilon \ := \ D_\varepsilon^* M_\rho^* H^\varepsilon M_\rho D_\varepsilon, \quad V_\varepsilon \ := \ D_\varepsilon^* M_\rho^* V^\varepsilon M_\rho D_\varepsilon \ = \ V_{\mathrm c} + D_\varepsilon^* W D_\varepsilon\,. $$

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

The leading order of H_ε will turn out to be the sum of $-\Delta_{\mathrm v} + V_{\mathrm c}(q, \cdot) + W(q, 0)$ and $-\varepsilon^2 \Delta_{\mathrm h}$ (for details on M_ρ and the expansion of H_ε see Lemmas 1 & 5 below). When $-\varepsilon^2 \Delta_{\mathrm h}$ 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 e.g. [34]).

We need that the family of q-dependent operators $-\Delta_{\mathrm{v}} + V_{\mathrm{c}}(q, \cdot) + W(q, 0)$ 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 $\mathcal{H}_{\mathrm{f}}(q) := L^2(N_q\mathcal{C}, d\nu)$ and $V_0(q, \nu) := V_{\mathrm{c}}(q, \nu) + W(q, 0)$. The selfadjoint operator $(H_{\mathrm{f}}(q), H^2(N_q\mathcal{C}, d\nu))$ defined by*

$$H_{\mathrm{f}}(q) \ := \ -\Delta_{\mathrm{v}} \ + \ V_0(q, .) \tag{22}$$

is called the fiber Hamiltonian. *Its spectrum is denoted by $\sigma\big(H_{\mathrm{f}}(q)\big)$.*

i) A function $E_{\mathrm{f}} : \mathcal{C} \to \mathbb{C}$ is called an energy band, *if $E_{\mathrm{f}}(q) \in \sigma\big(H_{\mathrm{f}}(q)\big)$ for all $q \in \mathcal{C}$. E_{f} is called* simple, *if $E_{\mathrm{f}}(q)$ is a simple eigenvalue for all $q \in \mathcal{C}$.*

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

$$E_{\mathrm{f}}(q) = I(q) \cap \sigma\big(H_{\mathrm{f}}(q)\big), \qquad \inf_{q \in \mathcal{C}} \mathrm{dist}\big(\sigma\big(H_{\mathrm{f}}(q)\big) \setminus E_{\mathrm{f}}(q), E_{\mathrm{f}}(q)\big) = c_{\mathrm{gap}}. \tag{23}$$

iii) Set $\langle \nu \rangle := \sqrt{1 + |\nu|^2} = \sqrt{1 + \overline{g}_{(q,0)}(\nu, \nu)}$. A separated energy band E_{f} is called a constraint energy band, *if there is $\Lambda_0 > 0$ such that the family of spectral projections $P_0 : \mathcal{C} \to \mathcal{L}\big(\mathcal{H}_{\mathrm{f}}(q)\big)$ corresponding to E_{f} satisfies*

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

We emphasize that condition ii) is known to imply condition iii) in lots of cases, for example for eigenvalues below the continuous spectrum (see [19] for a review of known results). Besides, condition ii) is a uniform but local condition (see Figure 3).

The family of spectral projections $P_0 : \mathcal{C} \to \mathcal{L}\big(\mathcal{H}_{\mathrm{f}}(q)\big)$ associated to a simple energy band E_{f} corresponds to a line bundle over $\mathcal{C}$. If this bundle has a global section $\varphi_{\mathrm{f}} : \mathcal{C} \to \mathcal{H}_{\mathrm{f}}(q)$ of normalized eigenfunctions, it holds for all $q \in \mathcal{C}$ that $(P_0 \psi)(q) = \langle \varphi_{\mathrm{f}} | \psi \rangle_{\mathcal{H}_{\mathrm{f}}(q)} \varphi_{\mathrm{f}}(q)$. Furthermore, φ_{f} can be used to
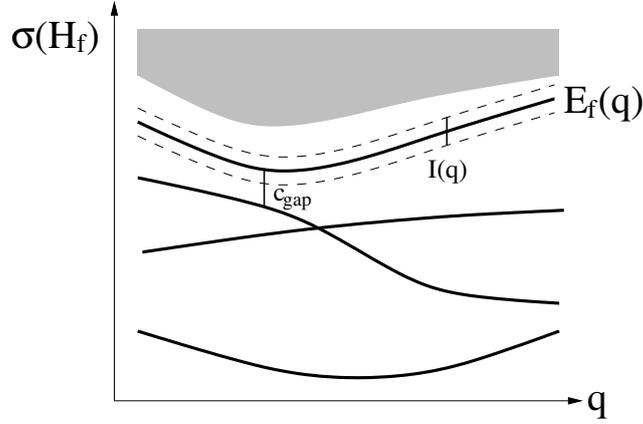
Figure 3: $E_\mathrm{f}(q)$ has to be separated by a local gap that is uniform in q.

define a unitary mapping U_0 between the corresponding subspace $P_0 \mathcal{H}$ and $L^2(\mathcal{C}, d\mu)$ by

$$(U_0\,\psi)(q) \;:=\; \langle \varphi_\mathrm{f} | \psi \rangle_{\mathcal{H}_\mathrm{f}(q)}.$$

So any $\psi \in P_0 \mathcal{H}$ has the product structure $\psi = (U_0 \psi) \varphi_\mathrm{f}$. Since V_0 and therefore φ_f 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 $[H_\varepsilon, P_0] = [-\varepsilon^2 \Delta_\mathrm{h}, P_0] + \mathcal{O}(\varepsilon)$ is of order ε. For long times this is a consequence of adiabatic decoupling.

On the macroscopic scale the corresponding eigenfunction $D_\varepsilon \varphi_\mathrm{f}$ 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 $\mathrm{e}^{-\Lambda_0 |\zeta|/\varepsilon}$. This is visualized in Figure 4.
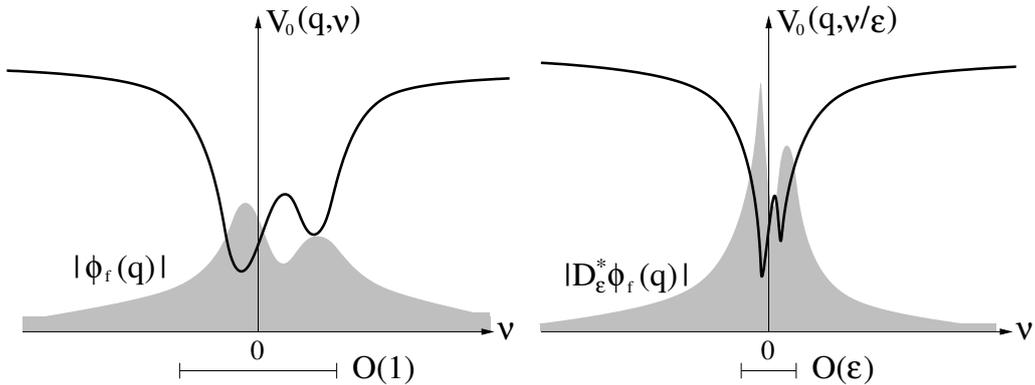

Figure 4: On the macroscopic level φ_f is localized on a scale of oder ε.

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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_{f} 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 [30] and Froese-Herbst [15], since [30] is the most general one on a theoretical physics level and [15] 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

$$\tilde{H}^\varepsilon = -\Delta_{N\mathcal{C}} + \varepsilon^{-2}V_{\mathrm{c}}^\varepsilon + W\,. \tag{24}$$

The confining potential $V_{\mathrm{c}}^\varepsilon$ 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 $R(q) \in \mathrm{SO}(k)$ such that

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

for some fixed point q_0 on $\mathcal{C}$. As a consequence, the eigenvalues of the resulting fiber Hamiltonian $H_{\mathrm{f}}(q) = -\Delta_{\mathrm{v}} + V_{\mathrm{c}}(q,\cdot)$ are constant, $E_{\mathrm{f}}(q) \equiv E_{\mathrm{f}}$. As our Theorems 1 and 2, the final result in [30] and somewhat disguised also in [15] 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 [15, 30] about (24) are related to our results on the seemingly different problem (21). 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 $\tilde{H}^\varepsilon$ by ε^2, the resulting Hamiltonian

$$\varepsilon^2\tilde{H}^\varepsilon = -\varepsilon^2\Delta_{N\mathcal{C}} + V_{\mathrm{c}}^\varepsilon + \varepsilon^2 W\,,$$

is the same as H^ε in (21), 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 (21) by ε^2, this should be interpreted in the following way. Results valid for times of order

one for the group generated by $\tilde{H}^\varepsilon$ 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 [15, 30] are valid on the same physical time scale as ours.

We look at (21) for initial data with horizontal kinetic energies $\langle \psi_0^\varepsilon | - \varepsilon^2 \Delta_{\mathrm{h}} \psi_0^\varepsilon \rangle$ of order one. This corresponds to horizontal kinetic energies $\langle \psi_0^\varepsilon | - \Delta_{\mathrm{h}} \psi_0^\varepsilon \rangle$ of order ε^{-2} in (24), i.e. to the situation where potential and kinetic energies are of the same order. However, in [15, 25, 30] 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 $\varepsilon^{-2} E_{\mathrm{f}}(q)$ given by the normal eigenvalue must be constant. This is achieved in [15, 25, 30] by assuming that, up to rotations, the confining potential is the same everywhere on $\mathcal{C}$.

Technically, the assumption that (in our units) $\langle \psi_0^\varepsilon | - \varepsilon^2 \Delta_{\mathrm{h}} \psi_0^\varepsilon \rangle$ 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},

$$\left\| \left[\mathrm{e}^{-\mathrm{i} H_\varepsilon t}, P_0 \right] \right\| = \mathcal{O}(\varepsilon^2 |t|).$$

To get approximate invariance for times of order ε^{-2} one needs an additional adiabatic argument. In [15] 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

$$\left\| \left[\mathrm{e}^{-\mathrm{i} H_\varepsilon t}, P_0 \right] \right\| = \mathcal{O}(\varepsilon |t|).$$

Therefore we need to replace the adiabatic subspaces $P_0 \mathcal{H}$ by so called super-adiabatic subspaces $P_\varepsilon \mathcal{H}$, for which $\left\| \left[\mathrm{e}^{-\mathrm{i} H_\varepsilon t}, P_\varepsilon \right] \right\| = \mathcal{O}(\varepsilon^3 |t|)$, 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 (24) 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 (21). 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 (24) the confining potential is scaled to the level of normal kinetic energies for ε-localized solutions, while in (21) 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 [25, 26, 30], and nanotubes and -films (see e.g. [6]). 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 (21).

2 Main results

2.1 Effective dynamics on the constraint manifold

Since the constraining 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 construct 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.

When there is a global orthonormal frame of the eigenspace bundle defined by $P_0(q)$, the dynamics inside the superadiabatic subspaces $P_\varepsilon\mathcal{H}$ can be mapped unitarily to dynamics on a space over the submanifold only.

Remark 1 *Let E_{f} be a simple constraint energy band (see Definition 3).*

i) Let the eigenspace bundle associated to E_{f} admit a smooth global section $\varphi_{\mathrm{f}} : \mathcal{C} \to \mathcal{H}_{\mathrm{f}}(q)$ of normalized eigenfunctions. Then the partial unitary operator $U_0 : \mathcal{H} \to L^2(\mathcal{C}, d\mu)$ defined by $(U_0\psi)(q) := \langle \varphi_{\mathrm{f}}(q, \cdot) | \psi(q, \cdot) \rangle_{\mathcal{H}_{\mathrm{f}}(q)}$ satisfies $U_0^* U_0 = P_0$ and $U_0 U_0^* = 1$, where U_0^* is given by $(U_0^*\psi)(q, \nu) = \varphi_{\mathrm{f}}(q, \nu)\psi(q)$.

ii) If $\mathcal{C}$ is contractible or if E_{f} is the ground state energy band of H_{f}, i.e. $E_{\mathrm{f}}(q) = \inf \sigma\big(H_{\mathrm{f}}(q)\big)$ for all $q \in \mathcal{C}$, then the associated eigenspace bundle has a smooth global section $\varphi_{\mathrm{f}} : \mathcal{C} \to \mathcal{H}_{\mathrm{f}}(q)$ of normalized eigenfunctions.

To see ii) we notice that, on the one hand, all bundles over a contractible manifold are trivializable. On the other hand, E_{f} has to be an eigenvalue for all q due to the gap condition and the eigenfunctions of $H_{\mathrm{f}}(q)$ can be chosen real-valued because $H_{\mathrm{f}}(q)$ is a real operator for all $q \in \mathcal{C}$. Furthermore, the groundstate of a Schrödinger operator with a bounded potential can always be chosen strictly positive (see [37]). This defines an orientation on the real eigenspace bundle and thus a trivialization on the real line bundle.

In the following, we restrict ourselves to a simple energy band, i.e. with one-dimensional eigenspaces because we do not want to overburden the result about the effective Hamiltonian (Theorem 2). To circumvent the possible non-triviality of the eigenspace bundle, we simply assume the existence of a trivializing frame for our main results.

Theorem 1 *Let $V_{\mathrm{c}}, W \in C_{\mathrm{b}}^{\infty}(\mathcal{C}, C_{\mathrm{b}}^{\infty}(N_q\mathcal{C}))$ and let E_{f} be any associated simple constraint energy band whose eigenspace bundle has a smooth section of normalized eigenfunctions.*
Then there are $C < \infty$ and $\varepsilon_0 > 0$ which satisfy that for all $\varepsilon < \varepsilon_0$ there are

- *a closed subspace $P^{\varepsilon}\overline{\mathcal{H}} \subset \overline{\mathcal{H}}$ with orthogonal projection P^{ε},*

- *a Riemannian metric $g_{\mathrm{eff}}^{\varepsilon}$ on $\mathcal{C}$ with associated measure $d\mu_{\mathrm{eff}}^{\varepsilon}$,*

- *$U^{\varepsilon} : \overline{\mathcal{H}} \to \mathcal{H}_{\mathrm{eff}} := L^2(\mathcal{C}, d\mu_{\mathrm{eff}}^{\varepsilon})$ with $U^{\varepsilon*}U^{\varepsilon} = P^{\varepsilon}$ and $U^{\varepsilon}U^{\varepsilon*} = 1$,*

such that $\big(H_{\mathrm{eff}}^{\varepsilon} := U^{\varepsilon}H^{\varepsilon}U^{\varepsilon*}, U^{\varepsilon}\mathcal{D}(H^{\varepsilon})\big)$ is self-adjoint on $\mathcal{H}_{\mathrm{eff}}$ and

$$\left\|\big(\mathrm{e}^{-\mathrm{i}H^{\varepsilon}t} - U^{\varepsilon*}\mathrm{e}^{-\mathrm{i}H_{\mathrm{eff}}^{\varepsilon}t}U^{\varepsilon}\big)P^{\varepsilon}\chi(H^{\varepsilon})\right\|_{\mathcal{L}(\overline{\mathcal{H}})} \leq C\,\varepsilon^3\,|t| \qquad (25)$$

for all $t \in \mathbb{R}$ and each Borel function $\chi : \mathbb{R} \to [-1, 1]$ with $\operatorname{supp}\chi \subset (-\infty, E]$. Here $\chi(H^{\varepsilon})$ is defined via the spectral theorem.

The proof of this result can be found in Section 3.1. The estimate (25) means that, after cutting off large energies, the superadiabatic subspace $P^{\varepsilon}\overline{\mathcal{H}}$ is invariant up to errors of order $\varepsilon^3|t|$ and that on this subspace of $\overline{\mathcal{H}}$ the unitary group $\mathrm{e}^{-\mathrm{i}H^{\varepsilon}t}$ is unitarily equivalent to the effective unitary group $\mathrm{e}^{-\mathrm{i}H_{\mathrm{eff}}^{\varepsilon}t}$ on $L^2(\mathcal{C}, d\mu_{\mathrm{eff}}^{\varepsilon})$ with the same error. In particular, there is adiabatic decoupling of the horizontal and vertical dynamics.

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 pointed out here that, while $P^\varepsilon\chi(H^\varepsilon)$ is not a projection, $\|P^\varepsilon\chi(H^\varepsilon)\psi\| \geq (1-c\varepsilon)\|\psi\|$ on the relevant sub-space $U^*\tilde\chi(H^\varepsilon_{\text{eff}})\mathcal{H}_{\text{eff}}$ for any $\tilde\chi$ with support at least slightly smaller than χ's and a $c < \infty$ independent of ε (this follows from Lemma 7 below).

Before we come to the form of the effective Hamiltonian, we state our result about effective dynamics for $\mathcal{A}$, which follows from the one above.

Definition 4 *Set $A\psi := \left(\frac{d\overline{\mu}}{\Phi^*d\tau}\right)^{-1/2}(\psi\circ\Phi)$ with $\Phi : N\mathcal{C} \to \mathcal{B}_\delta$ as constructed in Section 1.1 and $\Phi^*d\tau$ the pullback of $d\tau$ via Φ. This defines an operator $A \in \mathcal{L}\left(L^2(\mathcal{A},d\tau),\overline{\mathcal{H}}\right)$ 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 $H^\varepsilon_\mathcal{A} := -\varepsilon^2\Delta_\mathcal{A} + V^\varepsilon_\mathcal{A}$ be self-adjoint on $L^2(\mathcal{A},d\tau)$. Assume that $V^\varepsilon := AV^\varepsilon_\mathcal{A}A^*$ satisfies the assumptions from Theorem 1. Then there are $C < \infty$ and $\varepsilon_0 > 0$ such that*

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

for all $0 < \varepsilon \leq \varepsilon_0$, $t \in \mathbb{R}$, and each Borel function $\chi : \mathbb{R} \to [-1,1]$ with $\mathrm{supp}\,\chi \subset (-\infty, E]$.

The proof of this result can be found in Section 3.2. Of course, the choice of our metric (17) 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 range of 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 $V^\varepsilon_\mathcal{A}$, i.e. they only have to be valid on a tubular neighborhood of $\mathcal{C}$ with diameter δ. Furthermore, $V^\varepsilon := AV^\varepsilon_\mathcal{A}A^*$ is convergent for $|\nu| \to \infty$. 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

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

Theorem 2 *In addition to the assumptions of Theorem 1, assume that the global family of eigenfunctions φ_{f} associated to E_{f} is in $C_{\mathrm{b}}^{\infty}\big(\mathcal{C}, \mathcal{H}_{\mathrm{f}}(q)\big)$.*
For all ε small enough there is a self-adjoint operator $H_{\mathrm{eff}}^{(2)}$ on $\mathcal{H}_{\mathrm{eff}}$ such that for each Borel function $\chi : \mathbb{R} \to [-1,1]$ with $\operatorname{supp}\chi \subset (-\infty, E]$, for every $\xi \in \{U^{\varepsilon}\chi(H^{\varepsilon})U^{\varepsilon*}, \chi(H_{\mathrm{eff}}^{\varepsilon}), \chi(H_{\mathrm{eff}}^{(2)})\}$, and for all $\psi, \phi \in \mathcal{H}_{\mathrm{eff}}$ satisfying $\psi = \chi(-\varepsilon^2\Delta_{\mathcal{C}} + E_{\mathrm{f}})\psi$ it holds that $\| (H_{\mathrm{eff}}^{\varepsilon} - H_{\mathrm{eff}}^{(2)})\xi \|_{\mathcal{L}(\mathcal{H}_{\mathrm{eff}})} = \mathcal{O}(\varepsilon^3)$ and

$$
\begin{aligned}
\langle \phi \,| \, & H_{\mathrm{eff}}^{(2)} \psi \rangle_{\mathcal{H}_{\mathrm{eff}}} \\
&= \int_{\mathcal{C}} \Big(g_{\mathrm{eff}}^{\varepsilon}\big((p_{\mathrm{eff}}^{\varepsilon}\phi)^{*}, p_{\mathrm{eff}}^{\varepsilon}\psi\big) \,+\, \phi^{*}\big(E_{\mathrm{f}} + \varepsilon \,\langle \varphi_{\mathrm{f}}|(\nabla_{.}^{\mathrm{v}}W)\varphi_{\mathrm{f}}\rangle_{\mathcal{H}_{\mathrm{f}}} + \varepsilon^2\, W^{(2)}\big)\,\psi \\
&\qquad\qquad -\, \varepsilon^2\,\mathcal{M}\big(\Psi^{*}(\varepsilon\nabla p_{\mathrm{eff}}^{\varepsilon}\phi, p_{\mathrm{eff}}^{\varepsilon}\phi, \phi),\, \Psi(\varepsilon\nabla p_{\mathrm{eff}}^{\varepsilon}\psi, p_{\mathrm{eff}}^{\varepsilon}\psi, \psi)\big)\Big)\, d\mu_{\mathrm{eff}}^{\varepsilon},
\end{aligned}
$$

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

$$
\begin{aligned}
g_{\mathrm{eff}}^{\varepsilon}(\tau_1, \tau_2) &= g(\tau_1, \tau_2) \,+\, \varepsilon\,\langle \varphi_{\mathrm{f}} \,|\, 2\mathrm{II}(\,.\,)(\tau_1,\tau_2)\,\varphi_{\mathrm{f}}\rangle_{\mathcal{H}_{\mathrm{f}}} \\
&\quad + \varepsilon^2\,\Big\langle \varphi_{\mathrm{f}} \,\Big|\, 3g\big(\mathcal{W}(\,.\,)\tau_1, \mathcal{W}(\,.\,)\tau_2\big)\,\varphi_{\mathrm{f}} \,+\, \overline{\mathcal{R}}\big(\tau_1, \,.\,, \tau_2, \,.\,\big)\varphi_{\mathrm{f}}\Big\rangle_{\mathcal{H}_{\mathrm{f}}}, \\
p_{\mathrm{eff}}^{\varepsilon}\psi &= -\mathrm{i}\varepsilon\mathrm{d}\psi \,-\, \mathrm{Im}\,\Big(\varepsilon\,\langle \varphi_{\mathrm{f}}|\nabla^{\mathrm{h}}\varphi_{\mathrm{f}}\rangle_{\mathcal{H}_{\mathrm{f}}} \,-\, \varepsilon^2\int_{N_q\mathcal{C}} \tfrac{2}{3}\,\varphi_{\mathrm{f}}^{*}\,\overline{\mathrm{R}}(\nabla^{\mathrm{v}}\varphi_{\mathrm{f}}, \nu)\nu\, d\nu \\
&\qquad\qquad + \varepsilon^2\,\big\langle \varphi_{\mathrm{f}} \,\big|\, 2\big(\mathcal{W}(\,.\,) - \langle \varphi_{\mathrm{f}} | \mathcal{W}(\,.\,)\varphi_{\mathrm{f}}\rangle_{\mathcal{H}_{\mathrm{f}}}\big)\,\nabla^{\mathrm{h}}\varphi_{\mathrm{f}}\big\rangle_{\mathcal{H}_{\mathrm{f}}}\Big)\,\psi,
\end{aligned}
$$

with $\mathcal{W}$ the Weingarten mapping, II the second fundamental form, $\overline{\mathrm{R}}$ 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 '$.$' are integrated over the fibers.
Furthermore, $W^{(2)} = \langle \varphi_{\mathrm{f}}|\tfrac{1}{2}(\nabla_{\cdot,\cdot}^{\mathrm{v}}W)\varphi_{\mathrm{f}}\rangle_{\mathcal{H}_{\mathrm{f}}} + V_{\mathrm{BH}} + V_{\mathrm{geom}} + V_{\mathrm{amb}}$ and

$$
\begin{aligned}
V_{\mathrm{BH}} &= \int_{N_q\mathcal{C}} g_{\mathrm{eff}}^{\varepsilon}(\nabla^{\mathrm{h}}\varphi_{\mathrm{f}}^{*},\, (1-P_0)\nabla^{\mathrm{h}}\varphi_{\mathrm{f}})\, d\nu, \\
V_{\mathrm{geom}} &= -\tfrac{1}{4}\,\overline{g}(\eta, \eta) \,+\, \tfrac{1}{2}\,\kappa \,-\, \tfrac{1}{6}\,\big(\overline{\kappa} + \operatorname{tr}_{\mathcal{C}}\overline{\mathrm{Ric}} + \operatorname{tr}_{\mathcal{C}}\overline{\mathcal{R}}\big), \\
V_{\mathrm{amb}} &= \int_{N_q\mathcal{C}} \tfrac{1}{3}\,\overline{\mathcal{R}}\big(\nabla^{\mathrm{v}}\varphi_{\mathrm{f}}^{*}, \nu, \nabla^{\mathrm{v}}\varphi_{\mathrm{f}}, \nu\big)\, d\nu, \\
\mathcal{M}(\Phi^{*}, \Psi) &= \big\langle \Phi \,\big|\, (1-P_0)\big(H_{\mathrm{f}} - E_{\mathrm{f}}\big)^{-1}(1-P_0)\,\Psi \big\rangle_{\mathcal{H}_{\mathrm{f}}} \\
\Psi(A, p, \phi) &= -\varphi_{\mathrm{f}}\operatorname{tr}_{\mathcal{C}}\big(\mathcal{W}(\nu)A\big) \,-\, 2g_{\mathrm{eff}}^{\varepsilon}\big(\nabla^{\mathrm{h}}\varphi_{\mathrm{f}}^{*}, p\big) \,+\, \varphi_{\mathrm{f}}(\nabla_{\nu}^{\mathrm{v}}W)\phi
\end{aligned}
$$

with η the mean curvature vector, $\kappa, \overline{\kappa}$ the scalar curvatures of $\mathcal{C}$ and $\mathcal{A}$, and $\operatorname{tr}_{\mathcal{C}}\overline{\mathrm{Ric}}, \operatorname{tr}_{\mathcal{C}}\overline{\mathcal{R}}$ 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. One might wonder whether the complicated form of the effective Hamiltonian renders the result useless for practical purposes. However, as explained in the introduction, the possibly much lower dimension of $\mathcal{C}$ compared to that of $\mathcal{A}$ outweighs the more complicated form of the Hamiltonian. Moreover, the effective Hamiltonian is of a form that allows the use of semiclassical techniques for a further analysis. Finally, in practical applications typically only some of the terms appearing in the effective Hamiltonian are relevant. As an example we discuss the case of a quantum wave guide in Section 2.4. At this point we only add some general remarks concerning the numerous terms in H_{eff} and their consequences.

Remark 2   *i) If $\mathcal{C}$ is compact or contractible or if E_{f} is the ground state energy of H_{f}, the assumption $V_0 \in C_{\mathrm{b}}^{\infty}\big(\mathcal{C}, C_{\mathrm{b}}^{\infty}(N_q\mathcal{C})\big)$ implies the extra assumption that $\varphi_{\mathrm{f}} \in C_{\mathrm{b}}^{\infty}(\mathcal{C}, \mathcal{H}_{\mathrm{f}})$ (see Lemma 11 in Section 4.3). We do not know if this implication holds true in general, but expect this for all relevant applications.*

  ii) $\nabla_{\tau}^{\mathrm{eff}}\psi := (\mathrm{i}\, p_{\mathrm{eff}}^{\varepsilon}\psi)(\tau)$ is a metric connection on the trivial complex line bundle over $\mathcal{C}$ where ψ takes its values, a so-called Berry connection. It is flat because φ_{f} can be chosen real-valued locally which follows from H_{f}'s being real. The first order correction in $p_{\mathrm{eff}}^{\varepsilon}$ is the geometric generalization of the Berry term appearing in the Born-Oppenheimer setting. 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 [30].

  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 φ_{f} 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 (see [34]). However, $\mathcal{M}$ 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 the choice of φ_{f} but only on P_0.

  v) The existence of the geometric extra potential V_{geom} has been stressed in the literature, in particular as the origin of curvature-induced bound states in quantum wave guides (reviewed by Duclos and Exner in [12]).

In our setting, these are relevant for sending signals over long distances only (see Remark 4 below). The potential V_{amb} was also found in [30].

vi) *If $H_{\mathrm{eff}}^{(2)}$ was defined by the expression in the theorem, the statement would be wrong for $\xi = \chi(H_{\mathrm{eff}}^{(2)})$ because the fourth order term in $\mathcal{M}$ would be dominant. Therefore $\mathcal{M}$ is modified in the definition of $H_{\mathrm{eff}}^{(2)}$ so that the associated operator is bounded (see (51) below). However, when energies of $H_{\mathrm{eff}}^{(2)}$ are approximated by perturbation theory or the WKB method, that modification is of lower order as the leading order of a quasimode ψ satisfies $\psi = \chi(-\varepsilon^2\Delta_{\mathcal{C}} + E_{\mathrm{f}})\psi + \mathcal{O}(\varepsilon)$ for some χ.*

Using Theorem 2 we may exchange $H_{\mathrm{eff}}^{\varepsilon}$ with $H_{\mathrm{eff}}^{(2)}$ in Theorem 1. After replacing P^{ε} and U^{ε} by their leading order expressions, which adds a time-independent error of order ε, it is not difficult to derive the following result.

Corollary 2 *Fix $E < \infty$ and set $U_0^{\varepsilon} := U_0 D_{\varepsilon}^*$. Under the assumptions of Theorem 2 there are $C < \infty$ and $\varepsilon_0 > 0$ such that*

$$\left\| \left(\mathrm{e}^{-\mathrm{i}H^{\varepsilon}t} - U_0^{\varepsilon *}\mathrm{e}^{-\mathrm{i}H_{\mathrm{eff}}^{(2)}t}U_0^{\varepsilon} \right) U_0^{\varepsilon *}\chi(H_{\mathrm{eff}}^{(2)})U_0^{\varepsilon} \right\|_{\mathcal{L}(\overline{\mathcal{H}})} \leq C\,\varepsilon\,(\varepsilon^2|t| + 1) \qquad (26)$$

for all $0 < \varepsilon \leq \varepsilon_0$, $t \in \mathbb{R}$, and each Borel function $\chi : \mathbb{R} \to [-1,1]$ with $\mathrm{supp}\,\chi \subset (-\infty, E]$.

Corollary 2 will also be proved in Section 3.3. While (26) is somewhat weaker than (25), it is much better suited for applications, since U_0^{ε} is given in terms of the eigenfunction φ_{f} and depends on ε only via the dilation D_{ε}. So, in view of Theorem 2, all relevant expressions in (26) can be computed explicitly.

2.3 Approximation of eigenvalues

In this section we discuss in which way our effective Hamiltonian allows us to approximate certain parts of the discrete spectrum and the associated eigenfunctions of the original Hamiltonian. The following result shows how to obtain quasimodes of H^{ε} from the eigenfunctions of $H_{\mathrm{eff}}^{(2)}$ and vice versa.

Theorem 3 *Let E_{f} be a constraint energy band and $U^{\varepsilon}, H_{\mathrm{eff}}^{(2)}$ the operators associated to it via Theorems 1 & 2.*
a) Let $E \in \mathbb{R}$. Then there are $\varepsilon_0 > 0$ and $C < \infty$ such that for any family (E_{ε}) with $\limsup_{\varepsilon \to 0} E_{\varepsilon} < E$ and all $\varepsilon \leq \varepsilon_0$ the following implications hold:

i) $H_{\mathrm{eff}}^{(2)}\psi_{\varepsilon} = E_{\varepsilon}\psi_{\varepsilon} \quad \Longrightarrow \quad \| (H^{\varepsilon} - E_{\varepsilon})U^{\varepsilon *}\psi_{\varepsilon} \|_{\overline{\mathcal{H}}} \leq C\,\varepsilon^3\,\|U^{\varepsilon *}\psi_{\varepsilon}\|_{\overline{\mathcal{H}}},$

ii) $H^{\varepsilon}\psi^{\varepsilon} = E_{\varepsilon}\psi^{\varepsilon} \quad \Longrightarrow \quad \| (H_{\mathrm{eff}}^{(2)} - E_{\varepsilon})U^{\varepsilon}\psi^{\varepsilon} \|_{\mathcal{H}_{\mathrm{eff}}} \leq C\,\varepsilon^3\,\|\psi^{\varepsilon}\|_{\overline{\mathcal{H}}}.$

b) Let $E_\mathrm{f}(q) = \inf \sigma\big(H_\mathrm{f}(q)\big)$ for some (and thus for all) $q \in \mathcal{C}$ and define $E_1(q) := \inf \sigma\big(H_\mathrm{f}(q)\big) \setminus E_\mathrm{f}(q)$. Let a family (ψ^ε) with

$$\limsup_{\varepsilon \to 0} \big\langle \psi^\varepsilon \big| \big(-\varepsilon^2 M_\rho \Delta_\mathrm{v} M_\rho^* + V_0(q, \nu/\varepsilon) \big) \psi^\varepsilon \big\rangle \;<\; \inf_{q \in \mathcal{C}} E_1 \qquad (27)$$

be given. Then there are $\varepsilon_0 > 0$ and $c > 0$ such that $\| U^\varepsilon \psi^\varepsilon \|_{\mathcal{H}_\mathrm{eff}} \geq c \, \| \psi^\varepsilon \|_{\overline{\mathcal{H}}}$ for all $\varepsilon \leq \varepsilon_0$.

If one knows a priori that the spectrum of H^ε is discrete below the energy E, then statement a) i) implies, that H^ε has an eigenvalue in a interval of length $2C\varepsilon^3$ around E_ε. The statement b) ensures that a) ii) really yields a quasi-mode for normal energies below $\inf_{q \in \mathcal{C}} E_1$, i.e. that

$$H^\varepsilon \, \psi^\varepsilon \;=\; E_\varepsilon \psi^\varepsilon \quad \Longrightarrow \quad \| \, (H^{(2)}_\mathrm{eff} - E_\varepsilon) \, U^\varepsilon \psi^\varepsilon \, \|_{\mathcal{H}_\mathrm{eff}} \;\leq\; \tfrac{C}{c} \, \varepsilon^3 \, \| U^\varepsilon \psi^\varepsilon \|_{\mathcal{H}_\mathrm{eff}} \, .$$

Remark 3 *If the ambient manifold $\mathcal{A}$ is flat, $-\varepsilon^2 M_\rho \Delta_\mathrm{v} M_\rho^*$ is form-bounded by $-\varepsilon^2 \Delta_{N\mathcal{C}} + C\varepsilon^2$ for some $C < \infty$ independent of ε (this follows from Lemma 1 below and the expression (5.5) for $-\varepsilon^2 \Delta_{N\mathcal{C}}$ in [15]). Then, since $H^\varepsilon = -\varepsilon^2 \Delta_{N\mathcal{C}} + V_0(q, \nu/\varepsilon) + W(q, \nu) - W(q, 0)$, (27) follows from*

$$\limsup_{\varepsilon \to 0} \big\langle \psi^\varepsilon \big| H^\varepsilon \psi^\varepsilon \big\rangle \;<\; \inf_{q \in \mathcal{C}} E_1 - \sup_{(q, \nu)} \big(W(q, 0) - W(q, \nu) \big) \;=:\; E_*.$$

Therefore Theorem 3, in particular, implies that at least for flat $\mathcal{A}$ there is a one-to-one correspondence between the spectra of H^ε and $H^{(2)}_\mathrm{eff}$ below E_*.

One may ask whether a family (E_ε) of energies of H^ε with $\limsup E_\varepsilon < E_*$ exists at all. A sufficient condition is that $\sup_{(q,\nu)} \big(W(q,0) - W(q,\nu) \big)$ is strictly smaller than $\inf_{q \in \mathcal{C}} E_1 - \inf_{q \in \mathcal{C}} E_\mathrm{f}$. For this implies $\inf_{q \in \mathcal{C}} E_\mathrm{f} < E_*$, and the spectrum of $H^{(2)}_\mathrm{eff}$ in the interval $[\inf_{q \in \mathcal{C}} E_\mathrm{f}, E_*]$ has either a continuous part or the number of eigenvalues is at least of order ε^{-1} because $H^{(2)}_\mathrm{eff}$'s leading order term $-\varepsilon^2 \Delta_\mathcal{C} + E_\mathrm{f}$ is a semiclassical operator. Then by a) i) this is also true for H^ε.

The eigenvalues of $H^{(2)}_\mathrm{eff}$ can be approximated by the WKB construction, which is quite standard (see e.g. [18]). In the simplest case one obtains:

Corollary 3 *Denote by $E_\ell(A)$ the ℓ-th eigenvalue of a semi-bounded operator A, counted from the bottom of the spectrum.*
Let $\mathcal{A}$ be flat and let E_f be a constraint energy band with $\inf E_\mathrm{f} < E_*$ and $E_\mathrm{f}(q) = \inf \sigma\big(H_\mathrm{f}(q)\big)$ for all $q \in \mathcal{C}$. Assume that there is $q_0 \in \mathcal{C}$ such that $E_\mathrm{f}(q_0) < E_\mathrm{f}(q)$ for all $q \neq q_0$ and $\big(\nabla^2_{\partial_{x^i}, \partial_{x^j}} E_\mathrm{f} \big)(q_0)$ is positive definite.

Then for any $\ell \in \mathbb{N}$

$$E_\ell(H^\varepsilon) \;=\; E_{\mathrm{f}}(q_0) \,+\, \varepsilon E_\ell(H_{\mathrm{HO}}) \,+\, \mathcal{O}(\varepsilon^2),$$

where $H_{\mathrm{HO}} := -\Delta_{\mathbb{R}^d} + \frac{1}{2}(\nabla^2_{\partial_{x^i},\partial_{x^j}} E_{\mathrm{f}})(q_0)x^i x^j$ is a harmonic oscillator on $\mathbb{R}^d$.

We want to relate this to a result by Friedlander and Solomyak in [14]. There they consider the spectrum of the Dirichlet Laplacian $-\Delta_{\mathrm{D}}$ on the two-dimensional strip $\{(x,y) : x \in I,\, 0 < y < \varepsilon h(x)\}$ for any interval I and positive function h. They show that, if h has a global maxmimum at $q_0 \in I$ which is non-degenerate, then

$$E_\ell(-\varepsilon^2\Delta_{\mathrm{D}}) \;=\; \tilde{E}_{\mathrm{f}}(q_0) \,+\, \varepsilon E_\ell\big(-\partial^2_{xx} + \tfrac{1}{2}\tilde{E}''_{\mathrm{f}}(q_0)x^2\big) \,+\, o(\varepsilon),$$

where $\tilde{E}_{\mathrm{f}}(x) := \pi^2/h^2(x)$ is the lowest eigenvalue of the Dirichlet Laplacian on $[0, h(x)]$. So we would reproduce this result, if we were able to replace H_{f} by the Dirichlet Laplacian on a compact set of diameter ε. For a set with smooth boundary we do not see a problem in doing so. To the contrary, the strict localization to an ε-tube around $\mathcal{C}$ would simplify many steps in our proof considerably. Anyway, our result suggests that the result by Friedlander and Solomyak is true also for higher dimensions and when I is replaced by a curved space. Even more, it allows to conjecture the next corrections to the eigenvalues because it is straight forward to deduce the terms of order ε^2 from the expression of $H^{(2)}_{\mathrm{eff}}$ via standard perturbation theory.

2.4 Application to quantum wave guides

In this section we look at the special case of a curve $\mathcal{C}$ in $\mathcal{A} = \mathbb{R}^3$ equipped with the euclidean metric. Such curves may model quantum wave guides which have been discussed theoretically for long times but are nowadays also investigated experimentally. We will provide the expression for our effective Hamiltonian in this case and discuss which terms remain, if we add restrictions on the constraining potential or the geometry. Furthermore, we will apply Theorem 3 to obtain a statement about the spectrum of a twisted wave guide. For the sake of brevity, we assume that W, the non-constraining part of the potential, vanishes. Its contributions could be trivially added in all formulas and as long as $\sup_{(q,\nu)}\big(W(q,0) - W(q,\nu)\big)$ is small enough also in the statements (see the preceding subsection).

We first look at an infinite quantum wave guide. So let the curve $\mathcal{C}$ be given as a smooth injective $c : \mathbb{R} \to \mathbb{R}^3, x \mapsto c(x)$ that has bounded derivatives of any order and is parametrized by arc length ($|\dot{c}| = 1$). Wherever $\ddot{c} \neq 0$, the

Frenet frame of $T\mathcal{C} \times N\mathcal{C}$ is defined by $\tau := \dot{c}$, $\nu_1 := \ddot{c}/|\ddot{c}|$, and $\nu_2 := \tau \times \nu_1$. Wherever $\ddot{c} = 0$, we look at an arbitrary frame with $\tau := \dot{c}$ and $\nu_1 \cdot \dot{\nu}_2 = 0$. The (exterior) curvature of c is $\eta := |\ddot{c}|$ and its torsion is $\theta := -\nu_1 \cdot \dot{\nu}_2$. By the Frenet formulas the Weingarten mapping satisfies $\mathcal{W}(\nu_1) = \eta$ and $\mathcal{W}(\nu_2) = 0$ (see e.g. [7]). We denote the coordinates with respect to τ, ν_1, and ν_2 by x, n_1, and n_2 respectively. In these coordinates it holds $\nabla^{\mathrm{h}} = \partial_x + \theta(n_1 \partial_{n_2} - n_2 \partial_{n_1})$ (as can for example be seen from the general coordinate formula (75) below).

Now let E_{f} be a simple constraint energy band and φ_{f} a global family of eigenfunctions associated to it. We start by spelling out the formula for the effective Hamiltonian from Theorem 2. Of course, all terms containing the inner curvature of $\mathcal{C}$ and $\mathcal{A} = \mathbb{R}^3$ vanish due to the flatness of $\mathcal{C}$ and $\mathcal{A}$ with the euclidean metric. Since $\mathcal{C}$ is one-dimensional and contractible, φ_{f} can be chosen such that $p_{\mathrm{eff}}^{\varepsilon} \equiv -\mathrm{i}\varepsilon\partial_x$ globally. Then the effective Hamiltonian is

$$
\begin{aligned}
H_{\mathrm{qwg}}^{\varepsilon} = {} & -\varepsilon\partial_x\big(1 + \varepsilon\eta\langle\varphi_{\mathrm{f}}|n_1\varphi_{\mathrm{f}}\rangle + 3\varepsilon^2\eta^2\langle\varphi_{\mathrm{f}}|n_1^2\varphi_{\mathrm{f}}\rangle\big)\varepsilon\partial_x \;+\; E_{\mathrm{f}} \\
& -\varepsilon^2\eta^2/4 \;+\; \varepsilon^2\left(\langle\nabla^{\mathrm{h}}\varphi_{\mathrm{f}}|\nabla^{\mathrm{h}}\varphi_{\mathrm{f}}\rangle - |\langle\varphi_{\mathrm{f}}|\nabla^{\mathrm{h}}\varphi_{\mathrm{f}}\rangle|^2\right) \\
& + \varepsilon^2\left(4\,\varepsilon\partial_x\,\langle\nabla^{\mathrm{h}}\varphi_{\mathrm{f}}|R_{H_{\mathrm{f}}}(E_{\mathrm{f}})\nabla^{\mathrm{h}}\varphi_{\mathrm{f}}\rangle\,\varepsilon\partial_x\right. \\
& \qquad\quad + 4\,\eta\,\mathrm{Re}\,\varepsilon\partial_x\,\langle\nabla^{\mathrm{h}}\varphi_{\mathrm{f}}|R_{H_{\mathrm{f}}}(E_{\mathrm{f}})n_1\varphi_{\mathrm{f}}\rangle\,\varepsilon^2\partial_{xx}^2 \\
& \qquad\quad \left. + \eta^2\,\varepsilon^2\partial_{xx}^2\,\langle n_1\varphi_{\mathrm{f}}|R_{H_{\mathrm{f}}}(E_{\mathrm{f}})n_1\varphi_{\mathrm{f}}\rangle\,\varepsilon^2\partial_{xx}^2\right) \;+\; \mathcal{O}(\varepsilon^3) \quad (28)
\end{aligned}
$$

with $R_{H_{\mathrm{f}}}(E_{\mathrm{f}}) := (1 - P_0)(H_{\mathrm{f}} - E_{\mathrm{f}})^{-1}(1 - P_0)$ and $\langle\,\phi\,|\,\psi\,\rangle := \int_{\mathbb{R}^2}\phi^*\,\psi\,dn_1 dn_2$. We emphasize that formula (28) is only valid when applied to states with high energies cut off because this is required for the application of Theorem 2. In particular, this explains why the differential operator of fourth order is not to be thought of as the dominant term but only as of order ε^2. But still $\|\varepsilon\partial_x\psi\| \sim 1$ for a ψ of finite energy! Before we consider some special cases, we want to make the following crucial remark about sending signals through wave guides.

Remark 4 *For highly oscillating states ψ, i.e. with $\langle\psi| - \varepsilon^2\partial_{xx}^2\psi\rangle \sim 1$, the only term of order one besides $-\varepsilon^2\partial_{xx}^2$ is E_{f}. In particular, if E_{f} is constant, the dynamics is free at leading order and, even more, the potential terms are of order ε^2. So they only become relevant for times of order ε^{-2}. However, a semiclassical wave packet ψ covers distances of order ε^{-1} on this time scale. Hence, for such ψ note-worthy trapping occurs only for very long wave guides!*

If we consider a straight wave guide, i.e. $\eta \equiv 0$, the formula we end up with is a complete analogue of the one derived by Panati, Spohn, and Teufel in [34]

in the case of the Born-Oppenheimer approximation:

$$H_{\mathrm{qwg}}^{\varepsilon}|_{\eta \equiv 0} = -\varepsilon^2 \partial_{xx}^2 + E_{\mathrm{f}} + \varepsilon^2 \left(\langle \nabla^{\mathrm{h}} \varphi_{\mathrm{f}} | \nabla^{\mathrm{h}} \varphi_{\mathrm{f}} \rangle - |\langle \varphi_{\mathrm{f}} | \nabla^{\mathrm{h}} \varphi_{\mathrm{f}} \rangle|^2 \right)$$
$$+ \varepsilon^2 \, 4\varepsilon \partial_x \, \langle \nabla^{\mathrm{h}} \varphi_{\mathrm{f}} | R_{H_{\mathrm{f}}}(E_{\mathrm{f}}) \nabla^{\mathrm{h}} \varphi_{\mathrm{f}} \rangle \, \varepsilon \partial_x. \qquad (29)$$

We note that, although $\eta \equiv 0$, the x-dependence of the constraining potential still allows us to model interesting situations, e.g. a beam splitter [20].

Now we drop the assumption $\eta \equiv 0$ and assume that the constraining potential V_{c} is parallel with respect to ∇^{h} instead. This means $\nabla^{\mathrm{h}} V_{\mathrm{c}} \equiv 0$. Then we obtain a global family of eigenfunctions φ_{f} with $\nabla^{\mathrm{h}} \varphi_{\mathrm{f}} \equiv 0$ by taking it to be the parallel transport with respect to ∇^{h} of $\varphi_{\mathrm{f}}(q_0)$ for any $q_0 \in \mathcal{C}$. In addition, since V_{c} does not change its shape, E_{f} is constant and thus may be removed by redefining zero energy. Therefore we have

$$H_{\mathrm{qwg}}^{\varepsilon}|_{\nabla^{\mathrm{h}} V_{\mathrm{c}} \equiv 0} = -\varepsilon \partial_x \left(1 + \varepsilon \eta \langle \varphi_{\mathrm{f}} | n_1 \varphi_{\mathrm{f}} \rangle + 3\varepsilon^2 \eta^2 \langle \varphi_{\mathrm{f}} | n_1^2 \varphi_{\mathrm{f}} \rangle \right) \varepsilon \partial_x$$
$$- \varepsilon^2 \, \eta^2/4 \, + \, \varepsilon^2 \, \eta^2 \, \varepsilon^2 \partial_{xx}^2 \, \langle n_1 \varphi_{\mathrm{f}} | R_{H_{\mathrm{f}}}(E_{\mathrm{f}}) n_1 \varphi_{\mathrm{f}} \rangle \, \varepsilon^2 \partial_{xx}^2. \quad (30)$$

There is wide literature on quantum wave guides where the effects of bending and twisting on the spectrum of the Dirichlet Laplacian on an ε-tube with a fixed cross section is investigated (see the review [22] by Krejčiřík). If we consider the corresponding situation that V_{c} does not change its shape but is allowed to twist, E_{f} is the only term in (28) that may be neglected. Since the remaining potential terms are, however, of order ε^2, the kinetic energy operator $-\varepsilon^2 \partial_{xx}^2$ will also be of order ε^2 for low eigenvalues. So $H_{\mathrm{qwg}}^{\varepsilon}$ may be devided by ε^2. Keeping only the leading order terms we arrive at

$$H_{\mathrm{twist}}^{\varepsilon} := -\partial_{xx}^2 - \eta^2/4 + \langle \nabla^{\mathrm{h}} \varphi_{\mathrm{f}} | \nabla^{\mathrm{h}} \varphi_{\mathrm{f}} \rangle - |\langle \varphi_{\mathrm{f}} | \nabla^{\mathrm{h}} \varphi_{\mathrm{f}} \rangle|^2 \qquad (31)$$

The twisting assumption means that there is $\tilde{V}_{\mathrm{c}} \in C_{\mathrm{b}}^{\infty}(\mathbb{R}^2)$ and $\alpha \in C_{\mathrm{b}}^{\infty}(\mathbb{R})$ such that the constraining potential has the form:

$$\left(V_{\mathrm{c}}^{\alpha}(x) \right)(n_1, n_2) := \tilde{V}_{\mathrm{c}}\left(n_1 \cos \alpha(x) - n_2 \sin \alpha(x), n_1 \sin \alpha(x) + n_2 \cos \alpha(x) \right).$$

Then the family of eigenfunctions φ_{f} may be chosen as

$$\left(\varphi_{\mathrm{f}}(x) \right)(n_1, n_2) := \Phi_{\mathrm{f}}\left(n_1 \cos \alpha(x) - n_2 \sin \alpha(x), n_1 \sin \alpha(x) + n_2 \cos \alpha(x) \right)$$

for an eigenfunction Φ_{f} of $-\Delta_{\mathbb{R}^2} + \tilde{V}_{\mathrm{c}}(x)$ with eigenvalue E_{f}. We recall that $\nabla^{\mathrm{h}} = \partial_x + \theta(n_1 \partial_{n_2} - n_2 \partial_{n_1})$, where θ is the torsion of the curve. A lengthy but simple calculation yields

$$\langle \nabla^{\mathrm{h}} \varphi_{\mathrm{f}} | \nabla^{\mathrm{h}} \varphi_{\mathrm{f}} \rangle - |\langle \varphi_{\mathrm{f}} | \nabla^{\mathrm{h}} \varphi_{\mathrm{f}} \rangle|^2 = (\theta - \alpha')^2 \int_{\mathbb{R}^2} |n_1 \partial_{n_2} \Phi_{\mathrm{f}} - n_2 \partial_{n_1} \Phi_{\mathrm{f}}|^2 dn_1 dn_2.$$

We note that the integral is the expectation value of the squared angular momentum of Φ_{f} and thus vanishes for a rotation-invariant Φ_{f}. Now Theorem 3 together with Remark 3 implies the following result.

Corollary 4 *Denote by $E_\ell(A)$ the ℓ-th eigenvalue of a semi-bounded operator A, counted from the bottom of the spectrum.*
Let $\mathcal{C} \subset \mathbb{R}^3$ be an infinite curve, $W \equiv 0$, and E_f be a constraint energy band with $E_\mathrm{f}(q) = \inf \sigma\big(H_\mathrm{f}(q)\big)$ for all $q \in \mathcal{C}$. Let $L \in \mathbb{N}_0 \cup \{\infty\}$ be the number of eigenvalues of H_twist below the continuous spectrum, where H_twist is the following operator on $\mathbb{R}$:

$$H_\mathrm{twist} := -\partial_{xx}^2 - \eta^2/4 + C(\Phi_\mathrm{f})(\theta - \alpha')^2$$

with $C(\Phi_\mathrm{f}) := \int_{\mathbb{R}^2} |n_1 \partial_{n_2} \Phi_\mathrm{f} - n_2 \partial_{n_1} \Phi_\mathrm{f}|^2 dn_1 dn_2$.
If V_c only twists, i.e. $V_\mathrm{c} = V_\mathrm{c}^\alpha$ for some α as above, then for any $\ell < L$

$$E_\ell(H^\varepsilon) = E_\mathrm{f} + \varepsilon^2 E_\ell(H_\mathrm{twist}) + \mathcal{O}(\varepsilon^3).$$

This is an analogue of the result by Bouchitté, Mascarenhas and Trabucho in [5] for ε-tubes twisted by α. In [22] it was posed as an open problem to generalize this result to an infinite tube. Corollary 4 achieves this for a constraining potential that twists instead of the Dirchlet tube.

Up to now we have considered an infinite wave guide which is topological trivial. The only possible non-trivial topology for a one-dimensional manifold is that of a circle. So let $\mathcal{C}$ now be diffeomorphic to a circle. We refer to such a $\mathcal{C}$ as a *quantum wave circuit*. Because of the non-trivial topology our choices of the family φ_f made above are only possible locally but in general not globally. Therefore we rewrite (29) without those choices and ignoring the terms of order ε^2 for the moment:

$$H_\mathrm{qwc}^\varepsilon = p_\varepsilon^*\big(1 + \varepsilon\eta\langle\varphi_\mathrm{f}|n_1\varphi_\mathrm{f}\rangle\big)p_\varepsilon + E_\mathrm{f} + \mathcal{O}(\varepsilon^2) \tag{32}$$

with $p_\varepsilon = -\mathrm{i}\varepsilon\partial_x + \varepsilon\big\langle\varphi_\mathrm{f}\big|\mathrm{i}\big(\partial_x + \theta\,(n_1\partial_{n_2} - n_2\partial_{n_1})\big)\varphi_\mathrm{f}\big\rangle$. Although the curvature of the connection $\mathrm{i}p_\varepsilon$ always vanishes, it may have a non-trivial holonomy over the circle, which we will discuss next.

For the sake of simplicity we consider a round circle, i.e. with constant η and $\theta \equiv 0$. Let x be a 2π-periodic coordinate for it. The eigenfunction $\varphi_\mathrm{f}(x)$ can be chosen real-valued for each fixed x because H_f is real. This associates a real line bundle to E_f. From the topological point of view, there are two real line bundles over the sphere: the trivial one and the non-trivializable Möbius band. In the former case the global section φ_f can be chosen real everywhere. This implies $\langle\varphi_\mathrm{f}|\partial_x\varphi_\mathrm{f}\rangle \equiv 0$ which results in $\mathrm{i}p_\varepsilon = \varepsilon\partial_x$. Thus the holonomy group of $\mathrm{i}p_\varepsilon$ is trivial in this case. We will now provide an example for the realization of the Möbius band by a suitable constraining potential and show that the holonomy group of $\mathrm{i}p_\varepsilon$ becomes $\mathbb{Z}/2\mathbb{Z}$!

Let $\tilde{V}_c \in C_b^\infty(\mathbb{R}^2)$ have two orthogonal axes of reflection symmetry, i.e. in suitable coordinates

$$\tilde{V}_c(-N_1, N_2) \;=\; \tilde{V}_c(N_1, N_2) \;=\; \tilde{V}_c(N_1, -N_2). \tag{33}$$

Then the real ground state Φ_0 of $-\Delta_{\mathbb{R}^2} + \tilde{V}_c$ with energy E_0 is symmetric with respect to both reflections,

$$\Phi_0(N_1, N_2) \;=\; \Phi_0(-N_1, N_2) \;=\; \Phi_0(N_1, -N_2)\,,$$

while the first excited state Φ_1, also taken real-valued, with energy E_1 is typically only symmetric with respect to one reflection and anti-symmetric with respect to the other one, e.g.

$$\Phi_1(N_1, N_2) \;=\; -\,\Phi_1(-N_1, N_2) \;=\; \Phi_1(N_1, -N_2)\,. \tag{34}$$

This is true in particular for a harmonic oscillator with different frequencies (boundedness of $\tilde{V}_c$ is actually not important here). As the potential constraining to the round circle we choose the twisting potential V_c^α introduced above with $\alpha(x) = x/2$, i.e.

$$\big(V_c^{x/2}(x)\big)(n_1, n_2) \;:=\; \tilde{V}_c\big(\cos(x/2)n_1 - \sin(x/2)n_2, \sin(x/2)n_1 + \cos(x/2)n_2\big).$$

We note that due to (33) this defines a $V_c^{x/2} \in C_b^\infty\big(\mathcal{C}, C_b^\infty(N\mathcal{C})\big)$. Then

$$\big(\tilde{\varphi}_j(x)\big)(n_1, n_2) \;:=\; \Phi_j\big(\cos(x/2)n_1 - \sin(x/2)n_2, \sin(x/2)n_1 + \cos(x/2)n_2\big)$$

is an eigenfunction of $H_f(x) := -\Delta_v + V_c(x)$ with eigenvalue E_j for every x and $j \in \{0, 1\}$. However, while $\tilde{\varphi}_0$ is a smooth section of the corresponding eigenspace bundle, $\tilde{\varphi}_1$ is not. For by (34) it holds $\tilde{\varphi}_1(x) = -\tilde{\varphi}_1(x + 2\pi)$. Still the complex eigenspace bundle admits a smooth non-vanishing section. A possible choice is $\varphi_1(x) := e^{ix/2}\tilde{\varphi}_1(x)$. Using (34) we obtain that for the first excited band the effective Hamiltonian (32) reduces to

$$H_{\mathrm{qwc},1}^\varepsilon \;=\; E_1 \;+\; (-\mathrm{i}\varepsilon\partial_x + \varepsilon/2)^2 \;+\; \mathcal{O}(\varepsilon^2),$$

while for the ground state band it is

$$H_{\mathrm{qwc},0}^\varepsilon \;=\; E_0 \;-\; \varepsilon^2\partial_{xx}^2 \;+\; \mathcal{O}(\varepsilon^2)$$

This shows that depending on the symmetry of the normal eigenfunction the twist by an angle of π has different effects on the effective momentum operator in the effective Hamiltonian. With respect to the connection appearing in $H_{\mathrm{qwc},1}^\varepsilon$ the holonomy of a closed loop γ winding around the circle once is

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given by $h(\gamma) = \mathrm{e}^{\mathrm{i} \int_0^{2\pi} 1/2 \, dx} = -1$. Hence, the holonomy group of $\mathrm{i}p_\varepsilon$ is indeed $\mathbb{Z}/2\mathbb{Z}$ and the $1/2$ cannot be gauged away. Furthermore, a wave packet which travels around the circuit once accumulates a π-phase. This can be seen as an analogue of the Aharanov-Bohm effect, though with the only possible phase π.

The effect of this phase can also be seen in the level spacing of H_j^ε and thus, with Theorem 3, also in the spectrum of H^ε. The arguments that led to (31) for an infinite wave guide may be applied here, too, except that, of course, $-\partial_{xx}^2$ has to be replaced by $(-\mathrm{i}\partial_x + 1/2)^2$ for $H_{\mathrm{qwc},1}^\varepsilon$. Since η and $\alpha' - \theta$ are constant, the eigenvalues of $H_{\mathrm{qwc},1}^\varepsilon$ are

$$E_\ell(H_{\mathrm{qwc},1}^\varepsilon) = E_1 + \varepsilon^2 \left[(\ell + \tfrac{1}{2})^2 + \tfrac{C(\Phi_1) - 1}{4} \right] + \mathcal{O}(\varepsilon^3), \qquad \ell \in \mathbb{N}_0,$$

while for $H_{\mathrm{qwc},0}^\varepsilon$ we find

$$E_\ell(H_{\mathrm{qwc},0}^\varepsilon) = E_0 + \varepsilon^2 \left[\ell^2 + \tfrac{C(\Phi_0) - 1}{4} \right] + \mathcal{O}(\varepsilon^3), \qquad \ell \in \mathbb{N}_0.$$

Although a constraining potential that twists along a circle was investigated by Maraner in detail in [25] and by Mitchell in [30], the effect discussed above was not found in both treatments. The reason for this is that they allowed only for whole rotations and not for half ones to avoid the non-smoothness of $\tilde{\varphi}_1$. Finally, we note that it easy to generalize the statements above to a circuit whose curvature and potential twist are non-constant.

3 Proof of the main results

In the following, $\mathcal{L}(X, Y)$ is the Banach space of bounded operators between two Banach spaces X and Y. $\mathcal{D}(A)$ will *always denote the maximal domain* of an operator A, equipped with the graph norm. For convenience we set $\mathcal{D}(H^0) := \mathcal{H}$. A^* will always be used for the adjoint of A on $\mathcal{H}$ if not stated differently. 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 $\langle \nu \rangle^l$. Finally, we write $a \lesssim b$, if a is bounded by b times a constant independent of ε, and $a = \mathcal{O}(\varepsilon^l)$, if $\|a\| \lesssim \varepsilon^l$.

Throughout this section we assume that $V_{\mathrm{c}}, W \in C_{\mathrm{b}}^\infty(\mathcal{C}, C_{\mathrm{b}}^\infty(N\mathcal{C}))$ and that E_{f} is a constraint energy band as defined in Definition 3.

3.1 Proof of adiabatic decoupling

As explained in the introduction the first step in proving Theorem 1 is the unitary transformation of H^ε by multiplication with the square root of the

relative density $\rho := \frac{d\overline{\mu}}{d\mu \otimes d\nu}$ of the volume measure associated to $\overline{g}$ and the product measure on $N\mathcal{C}$. This transformation factorizes the measure, which will allow us to easily split the integral over $N\mathcal{C}$ later on, but it also yields an additional potential term. 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*

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

Then M_ρ is unitary and it holds

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

with $\Delta_{d\sigma_i} := \mathrm{div}_{d\sigma_i}\mathrm{grad}\,\psi$, where $\mathrm{grad}\,\psi$ is the vector field associated to $\mathrm{d}\psi$ via g and $\mathrm{div}_{d\sigma_i}$ 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 (19) that $\rho = \frac{d\overline{\mu}}{d\mu \otimes d\nu}$ is in $C_{\mathrm{b}}^\infty(N\mathcal{C})$ and strictly positive. Therefore V_ρ is in $C_{\mathrm{b}}^\infty(N\mathcal{C})$ for our choice of ρ. Since ρ is equal to 1 outside of $\mathcal{B}_\delta$, V_ρ is even in $C_{\mathrm{b}}^\infty(\mathcal{C}, C_{\mathrm{b}}^\infty(N_q\mathcal{C}))$ which coincides with $C_{\mathrm{b}}^\infty(N\mathcal{C})$ inside $\mathcal{B}_r$ for any $r < \infty$.

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 approximately commutes with H_ε:

Lemma 2 *Under the assumptions of Theorem 1 there is $\varepsilon_0 > 0$ such that for all $\varepsilon < \varepsilon_0$ there are an orthogonal projection $P_\varepsilon \in \mathcal{L}(\mathcal{H})$ and a unitary $\tilde{U}_\varepsilon \in \mathcal{L}(\mathcal{H})$ with $P_\varepsilon = \tilde{U}_\varepsilon^* P_0 \tilde{U}_\varepsilon$ and*

- $\|\tilde{U}_\varepsilon - 1\|_{\mathcal{L}(\mathcal{H})} = \mathcal{O}(\varepsilon), \quad \|P_\varepsilon\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon^m))} \lesssim 1,$
- $\|\langle\nu\rangle^l P_\varepsilon \langle\nu\rangle^j\|_{\mathcal{L}(\mathcal{H})} \lesssim 1, \quad \|\langle\nu\rangle^l P_\varepsilon \langle\nu\rangle^j\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon))} \lesssim 1,$
- $\|[H_\varepsilon, P_\varepsilon]\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon^m), \mathcal{D}(H_\varepsilon^{m-1}))} = \mathcal{O}(\varepsilon),$
- $\|[H_\varepsilon, P_\varepsilon]\chi(H_\varepsilon)\|_{\mathcal{L}(\mathcal{H}, \mathcal{D}(H_\varepsilon^m))} = \mathcal{O}(\varepsilon^3)$ (35)

for all $j, l, m \in \mathbb{N}_0$ and each Borel function $\chi : \mathbb{R} \to [-1, 1]$ satisfying $\mathrm{supp}\,\chi \subset (-\infty, E]$.

The construction of P_ε and $\tilde{U}_\varepsilon$ is carried out in Section 4.3. There is a heuristic discussion at the beginning of that section that the reader may find instructive to get an idea why P_ε and $\tilde{U}_\varepsilon$ exist. When we take its existence for granted, it is not difficult to prove that the effectice 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 we define by the expression in Theorem 2. For any fixed $E < \infty$, Lemma 2 yields some unitary $\tilde{U}_\varepsilon$ 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 $U_\varepsilon^* U_\varepsilon = \tilde{U}_\varepsilon^* U_0^* U_0 \tilde{U}_\varepsilon = \tilde{U}_\varepsilon^* P_0 \tilde{U}_\varepsilon = P_\varepsilon$ and

$$U_\varepsilon U_\varepsilon^* = U_0 \tilde{U}_\varepsilon \tilde{U}_\varepsilon^* U_0^* = U_0 U_0^* = 1. \tag{36}$$

In view of Lemma 1, we next set $U^\varepsilon := M_{\tilde{\rho}}^* U_\varepsilon D_\varepsilon^* M_\rho^*$ with $\rho := \frac{d\overline{\mu}}{d\mu \otimes d\nu}$ and $\tilde{\rho} := \frac{d\mu}{d\mu_{\text{eff}}^\varepsilon}$. In view of (36), the unitarity of $M_{\tilde{\rho}}$, M_ρ, and D_ε implies $U^\varepsilon U^{\varepsilon*} = 1$. Furthermore, we simply define P^ε by $P^\varepsilon := U^{\varepsilon*} U^\varepsilon$. Then U^ε is unitary from $P^\varepsilon \mathcal{H}$ to $L^2(\mathcal{C}, d\mu_{\text{eff}}^\varepsilon)$. Finally, we set

$$H_{\text{eff}}^\varepsilon := U^\varepsilon H^\varepsilon U^{\varepsilon*} = M_{\tilde{\rho}} U_\varepsilon H_\varepsilon U_\varepsilon^* M_{\tilde{\rho}}^*. \tag{37}$$

We notice that $H_{\text{eff}}^\varepsilon$ is symmetric by definition. Since $M_{\tilde{\rho}}$ is unitary and U_ε is unitary when restricted to $P_\varepsilon \mathcal{H}$ due to Lemma 2, the self-adjointness of $\left(H_{\text{eff}}^\varepsilon, U^\varepsilon \mathcal{D}(H^\varepsilon)\right)$ on $\mathcal{H}_{\text{eff}} := L^2(\mathcal{C}, d\mu_{\text{eff}}^\varepsilon)$ is implied by the self-adjointness of $\left(P_\varepsilon H_\varepsilon P_\varepsilon, P_\varepsilon \mathcal{D}(H_\varepsilon)\right)$ on $P_\varepsilon \mathcal{H}$, which is in turn a consequence of the self-adjointness of $\left(P_\varepsilon H_\varepsilon P_\varepsilon + (1-P_\varepsilon)H_\varepsilon(1-P_\varepsilon), \mathcal{D}(H_\varepsilon)\right)$ on $\mathcal{H}$. For ε small enough this last self-adjointness can be verified using Lemma 2 and the Kato-Rellich theorem (see e.g. [36]):

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

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 nescessary) the difference above is operator-bounded by H_ε with relative bound smaller than one. Now the Kato-Rellich theorem yields the claim, because $\left(H_\varepsilon, \mathcal{D}(H_\varepsilon)\right)$ is self-adjoint (as it is unitarily equivalent to the self-adjoint H^ε).

We now turn to the derivation of the estimate (25). To do so we first pull out the unitaries $M_{\tilde{\rho}}$, M_ρ and D_ε. Using that $D_\varepsilon^* M_\rho^* \chi(H^\varepsilon) D_\varepsilon M_\rho = \chi(D_\varepsilon^* M_\rho^* H^\varepsilon D_\varepsilon M_\rho) = \chi(H_\varepsilon)$ due to the spectral theorem we obtain by a straight forward calculation that

$$\begin{aligned}
&\left(\mathrm{e}^{-\mathrm{i}H^\varepsilon t} - U^{\varepsilon*} \mathrm{e}^{-\mathrm{i}H_{\text{eff}} t} U^\varepsilon\right) P^\varepsilon \chi(H^\varepsilon) \\
&= M_\rho D_\varepsilon \left(\mathrm{e}^{-\mathrm{i}H_\varepsilon t} - U_\varepsilon^* \mathrm{e}^{-\mathrm{i}U_\varepsilon H_\varepsilon U_\varepsilon^* t} U_\varepsilon\right) U_\varepsilon^* U_\varepsilon \chi(H_\varepsilon) D_\varepsilon^* M_\rho^*.
\end{aligned}$$

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 $U_\varepsilon U_\varepsilon^* = 1$ and $P_\varepsilon = U_\varepsilon^* U_\varepsilon$ we have that

$$
\begin{aligned}
\big(&\mathrm{e}^{-\mathrm{i}H_\varepsilon t} - U_\varepsilon^* \mathrm{e}^{-\mathrm{i}U_\varepsilon H_\varepsilon U_\varepsilon^* t} U_\varepsilon \big) U_\varepsilon^* U_\varepsilon \, \chi(H_\varepsilon) \\
&= \big(P_\varepsilon - U_\varepsilon^* \mathrm{e}^{-\mathrm{i}U_\varepsilon H_\varepsilon U_\varepsilon^* t} U_\varepsilon \mathrm{e}^{\mathrm{i}H_\varepsilon t} \big) \mathrm{e}^{-\mathrm{i}H_\varepsilon t} \, \chi(H_\varepsilon) + \big[\mathrm{e}^{-\mathrm{i}H_\varepsilon t}, P_\varepsilon \big] \chi(H_\varepsilon) \\
&= \mathrm{i} \int_0^t U_\varepsilon^* \mathrm{e}^{-\mathrm{i}U_\varepsilon H_\varepsilon U_\varepsilon^* s} \big(U_\varepsilon H_\varepsilon U_\varepsilon^* U_\varepsilon - U_\varepsilon H_\varepsilon \big) \mathrm{e}^{\mathrm{i}H_\varepsilon s} \, ds \, \mathrm{e}^{-\mathrm{i}H_\varepsilon t} \, \chi(H_\varepsilon) \\
&\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad + \big[\mathrm{e}^{-\mathrm{i}H_\varepsilon t}, P_\varepsilon \big] \chi(H_\varepsilon) \\
&= \mathrm{i} \int_0^t U_\varepsilon^* \mathrm{e}^{-\mathrm{i}U_\varepsilon H_\varepsilon U_\varepsilon^* s} U_\varepsilon \big(H_\varepsilon P_\varepsilon - P_\varepsilon H_\varepsilon \big) \chi(H_\varepsilon) \, \mathrm{e}^{\mathrm{i}H_\varepsilon s} \, ds \, \mathrm{e}^{-\mathrm{i}H_\varepsilon t} \\
&\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad + \big[\mathrm{e}^{-\mathrm{i}H_\varepsilon t}, P_\varepsilon \big] \chi(H_\varepsilon), \quad (38)
\end{aligned}
$$

where we used that $[\mathrm{e}^{-\mathrm{i}H_\varepsilon s}, \chi(H_\varepsilon)] = 0$ for any s due to the spectral theorem. Now we observe that (35) implies that

$$
\big\| \big[\mathrm{e}^{-\mathrm{i}H_\varepsilon t}, P_\varepsilon \big] \chi(H_\varepsilon) \big\|_{\mathcal{L}(\mathcal{H})} = \mathcal{O}(\varepsilon^3 |t|), \tag{39}
$$

as it holds

$$
\begin{aligned}
\big[\mathrm{e}^{-\mathrm{i}H_\varepsilon t}, P_\varepsilon \big] \chi(H_\varepsilon) &= \mathrm{e}^{-\mathrm{i}H_\varepsilon t} \big(P_\varepsilon - \mathrm{e}^{\mathrm{i}H_\varepsilon t} P_\varepsilon \mathrm{e}^{-\mathrm{i}H_\varepsilon t} \big) \chi(H_\varepsilon) \\
&= -\mathrm{e}^{-\mathrm{i}H_\varepsilon t} \, \mathrm{i} \int_0^t \mathrm{e}^{\mathrm{i}H_\varepsilon s} \big(H_\varepsilon P_\varepsilon - P_\varepsilon H_\varepsilon \big) \mathrm{e}^{-\mathrm{i}H_\varepsilon s} \, ds \, \chi(H_\varepsilon) \\
&= -\mathrm{e}^{-\mathrm{i}H_\varepsilon t} \, \mathrm{i} \int_0^t \mathrm{e}^{\mathrm{i}H_\varepsilon s} [H_\varepsilon, P_\varepsilon] \chi(H_\varepsilon) \mathrm{e}^{-\mathrm{i}H_\varepsilon s} \, ds \overset{(35)}{=} \mathcal{O}(\varepsilon^3 |t|)
\end{aligned}
$$

because of Lemma 2 and $\|\mathrm{e}^{-\mathrm{i}H_\varepsilon s}\|_{\mathcal{L}(\mathcal{H})} = 1$ for any s. So, in view of (38),

$$
\begin{aligned}
\big\| \big(&\mathrm{e}^{-\mathrm{i}H_\varepsilon t} - U_\varepsilon^* \mathrm{e}^{-\mathrm{i}U_\varepsilon H_\varepsilon U_\varepsilon^* t} U_\varepsilon \big) P_\varepsilon \, \chi(H_\varepsilon) \big\|_{\mathcal{L}(\mathcal{H})} \\
&\overset{(39)}{\leq} \left\| \int_0^t U_\varepsilon^* \mathrm{e}^{-\mathrm{i}U_\varepsilon H_\varepsilon U_\varepsilon^* s} U_\varepsilon \big[H_\varepsilon, P_\varepsilon \big] \chi(H_\varepsilon) \, \mathrm{e}^{\mathrm{i}H_\varepsilon s} \, ds \right\|_{\mathcal{L}(\mathcal{H})} + \mathcal{O}(\varepsilon^3 |t|) \\
&\leq |t| \underbrace{\big\| U_\varepsilon^* \mathrm{e}^{-\mathrm{i}U_\varepsilon H_\varepsilon U_\varepsilon^* s} U_\varepsilon \big\|_{\mathcal{L}(\mathcal{H})}}_{\leq 1} \big\| \big[H_\varepsilon, P_\varepsilon \big] \chi(H_\varepsilon) \big\|_{\mathcal{L}(\mathcal{H})} + \mathcal{O}(\varepsilon^3 |t|) \\
&\overset{(35)}{=} \mathcal{O}(\varepsilon^3 |t|).
\end{aligned}
$$

This proves the error estimate (25). $\qquad\qquad\qquad\qquad\qquad\qquad\square$

PROOF OF LEMMA 1:
M_ρ is an isometry because for all $\psi, \varphi \in L^2(\mathcal{M}, d\sigma_2)$

$$
\int_{\mathcal{M}} M_\rho \psi^* \, M_\rho \varphi \, d\sigma_1 = \int_{\mathcal{M}} \psi^* \, \varphi \, \rho^{-1} \, d\sigma_1 = \int_{\mathcal{M}} \psi^* \, \varphi \, d\sigma_2.
$$

Therefore it is clear that
$$M_\rho^* \psi \;=\; \rho^{\frac{1}{2}} \psi$$
which is well-defined because ρ is positive. One immediately concludes
$$M_\rho M_\rho^* \;=\; 1 \;=\; M_\rho^* M_\rho$$
and thus M_ρ is unitary. Now we note that $[\mathrm{grad}, \rho^{-\frac{1}{2}}] = -\frac{1}{2}\,\rho^{-\frac{1}{2}}\,\mathrm{grad}\ln\rho$.
So we have

$$
\begin{aligned}
M_\rho(-\Delta_{d\sigma_1})M_\rho^*\psi \;&=\; -\rho^{\frac{1}{2}}\mathrm{div}_{d\sigma_1}\,\mathrm{grad}(\rho^{-\frac{1}{2}}\psi)\\
&=\; -\rho^{\frac{1}{2}}\mathrm{div}_{d\sigma_1}\,\rho^{-\frac{1}{2}}\big(\mathrm{grad}\psi - \tfrac{1}{2}(\mathrm{grad}\ln\rho)\psi\big)\\
&=\; -\rho^{\frac{1}{2}}\mathrm{div}_{d\sigma_1}\,\rho^{-\frac{1}{2}}\,\mathrm{grad}\psi \;+\; \rho^{\frac{1}{2}}\mathrm{div}_{d\sigma_1}\Big(\rho^{-\frac{1}{2}}\tfrac{1}{2}(\mathrm{grad}\ln\rho)\psi\Big)
\end{aligned}
$$

On the one hand,
$$\rho^{\frac{1}{2}}\mathrm{div}_{d\sigma_1}\,\rho^{-\frac{1}{2}}\,\mathrm{grad}\psi \;=\; \rho\,\mathrm{div}_{d\sigma_1}\,\rho^{-1}\,\mathrm{grad}\psi \;+\; \tfrac{1}{2}\,g(\mathrm{grad}\ln\rho, \mathrm{grad}\psi)$$

and on the other hand,
$$
\begin{aligned}
\rho^{\frac{1}{2}}\mathrm{div}_{d\sigma_1}\Big(\rho^{-\frac{1}{2}}\tfrac{1}{2}(\mathrm{grad}\ln\rho)\psi\Big) \;=\; &-\tfrac{1}{4}\,g(\mathrm{grad}\ln\rho, \mathrm{grad}\ln\rho)\psi\\
&+\tfrac{1}{2}\,(\mathrm{div}_{d\sigma_1}\,\mathrm{grad}\ln\rho)\psi\\
&+\tfrac{1}{2}\,g(\mathrm{grad}\ln\rho, \mathrm{grad}\,\psi).
\end{aligned}
$$

Together we obtain
$$
\begin{aligned}
M_\rho(-\Delta_{d\sigma_1})M_\rho^*\psi \;=\; &-\rho\,\mathrm{div}_{d\sigma_1}\,\rho^{-1}\,\mathrm{grad}\psi\\
&-\Big(\tfrac{1}{4}\,g(\mathrm{grad}\ln\rho, \mathrm{grad}\ln\rho) - \tfrac{1}{2}\,\mathrm{div}_{d\sigma_1}\,\mathrm{grad}\ln\rho\Big)\psi\\
=\; &-\Delta_{d\sigma_2}\psi - \Big(\tfrac{1}{4}\,g(\mathrm{grad}\ln\rho, \mathrm{grad}\ln\rho) - \tfrac{1}{2}\Delta_{d\sigma_1}\ln\rho\Big)\psi,
\end{aligned}
$$

which is the claim. $\qquad\square$

3.2 Pullback of the results to the ambient space

In this section we show how to derive the corollary about effective dynamics on the ambient manifold $\mathcal{A}$ from Theorem 1. To do so we first state some immediate consequences of Lemma 2 for P^ε and U^ε from Theorem 1.

Corollary 5 *For ε small enough P^ε and U^ε from Theorem 1 satisfy*

- $\|P^\varepsilon\|_{\mathcal{L}(\mathcal{D}(H^{\varepsilon m}))} \lesssim 1$,
- $\|\langle \nu/\varepsilon \rangle^l P^\varepsilon \langle \nu/\varepsilon \rangle^j\|_{\mathcal{L}(\overline{\mathcal{H}})} \lesssim 1$, $\quad \|\langle \nu/\varepsilon \rangle^l P^\varepsilon \langle \nu/\varepsilon \rangle^j\|_{\mathcal{L}(\mathcal{D}(H^\varepsilon))} \lesssim 1$,
- $\|[H^\varepsilon, P^\varepsilon]\|_{\mathcal{L}(\mathcal{D}(H^{\varepsilon m+1}), \mathcal{D}(H^{\varepsilon m}))} = \mathcal{O}(\varepsilon)$, $\hfill (40)$
- $\|[H^\varepsilon, P^\varepsilon]\chi(H^\varepsilon)\|_{\mathcal{L}(\overline{\mathcal{H}}, \mathcal{D}(H^{\varepsilon m}))} = \mathcal{O}(\varepsilon^3)$, $\hfill (41)$
- $\|U^\varepsilon\|_{\mathcal{L}(\mathcal{D}(H^{\varepsilon m}), \mathcal{D}(H^{\varepsilon m}_{\mathrm{eff}}))} \lesssim 1$, $\quad \|U^{\varepsilon*}\|_{\mathcal{L}(\mathcal{D}(H^{\varepsilon m}_{\mathrm{eff}}), \mathcal{D}(H^{\varepsilon m}))} \lesssim 1$ $\hfill (42)$

for all $j, l, m \in \mathbb{N}_0$ and each Borel functions $\chi : \mathbb{R} \to [-1, 1]$ satisfying $\operatorname{supp}\chi \subset (-\infty, E]$.

The proof can be found at the end of this subsection. Now we gather some facts about the operator A defined in (4) and its adjoint.

Lemma 3 *Let A be defined by $A\psi := (\frac{d\overline{\mu}}{\Phi^* d\tau})^{-\frac{1}{2}} (\psi \circ \Phi)$ with $\Phi : N\mathcal{C} \to \mathcal{B}$ as constructed in Section 1.1.*
i) It holds $A \in \mathcal{L}(L^2(\mathcal{A}, d\tau), \overline{\mathcal{H}})$ with

$$\|A\psi\|_{L^2(N\mathcal{C}, d\overline{\mu})} \leq \|\psi\|_{L^2(\mathcal{A}, d\tau)} \qquad \forall\, \psi \in L^2(\mathcal{A}, d\tau).$$

ii) For $\varphi \in \overline{\mathcal{H}}$ the adjoint $A^* \in \mathcal{L}(\overline{\mathcal{H}}, L^2(\mathcal{A}, d\tau))$ of A is given by

$$A^*\varphi = \begin{cases} \left((\frac{d\overline{\mu}}{\Phi^* d\tau})^{\frac{1}{2}} \varphi\right) \circ \Phi^{-1} & \text{on } \mathcal{B}, \\ 0 & \text{on } \mathcal{A} \setminus \mathcal{B}. \end{cases}$$

It satisfies $\|A^*\varphi\|_{L^2(\mathcal{A}, d\tau)} = \|\varphi\|_{L^2(N\mathcal{C}, d\overline{\mu})}$, $A^*A = \chi_\mathcal{B}$, and $AA^* = 1$.
iii) It holds $A^* P^\varepsilon \in \mathcal{L}(\mathcal{D}(H^\varepsilon), \mathcal{D}(H^\varepsilon_\mathcal{A}))$ and

$$\|(H^\varepsilon_\mathcal{A} A^* - A^* H^\varepsilon) P^\varepsilon\|_{\mathcal{L}(\mathcal{D}(H^\varepsilon), L^2(\mathcal{A}, d\tau))} \lesssim \varepsilon^3. \hfill (43)$$

The last estimate is crucial for the proof of Corollary 1. It results from the two facts that $H^\varepsilon_\mathcal{A} A^* = A^* H^\varepsilon$ on $\mathcal{B}_{\delta/2}$ by construction and that 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

$$\left(\mathrm{e}^{-iH^\varepsilon_\mathcal{A} t} - A^* U^{\varepsilon*} \mathrm{e}^{-iH^\varepsilon_{\mathrm{eff}} t} U^\varepsilon A\right) A^* P^\varepsilon \chi(H^\varepsilon) A$$
$$= \left(\left(\mathrm{e}^{-iH^\varepsilon_\mathcal{A} t} A^* - A^* \mathrm{e}^{-iH^\varepsilon t}\right) + A^*\left(\mathrm{e}^{-iH^\varepsilon t} - U^{\varepsilon*} \mathrm{e}^{-iH^\varepsilon_{\mathrm{eff}} t} U^\varepsilon\right)\right) P^\varepsilon \chi(H^\varepsilon) A$$

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 (41) implies $[\mathrm{e}^{-\mathrm{i} H^\varepsilon t}, P^\varepsilon] \chi(H^\varepsilon) = \mathcal{O}(\varepsilon^3 |t|)$ analogously with the proof of (39). So

$$
\begin{aligned}
&(\mathrm{e}^{-\mathrm{i} H^\varepsilon_{\mathcal{A}} t} A^* - A^* \, \mathrm{e}^{-\mathrm{i} H^\varepsilon t}) P^\varepsilon \chi(H^\varepsilon) A \\
&\quad = \quad \mathrm{e}^{-\mathrm{i} H^\varepsilon_{\mathcal{A}} t} \big(A^* P^\varepsilon - \mathrm{e}^{\mathrm{i} H^\varepsilon_{\mathcal{A}} t} A^* \, P^\varepsilon \mathrm{e}^{-\mathrm{i} H^\varepsilon t} \big) \chi(H^\varepsilon) A \; + \; A^* [\mathrm{e}^{-\mathrm{i} H^\varepsilon t}, P^\varepsilon] \, \chi(H^\varepsilon) A \\
&\quad = \quad \mathrm{i} \mathrm{e}^{-\mathrm{i} H^\varepsilon_{\mathcal{A}} t} \int_0^t \mathrm{e}^{\mathrm{i} H^\varepsilon_{\mathcal{A}} s} \, (A^* P^\varepsilon H^\varepsilon - H^\varepsilon_{\mathcal{A}} A^* P^\varepsilon \, \chi(H^\varepsilon)) \, \mathrm{e}^{-\mathrm{i} H_\varepsilon s} \, A \, ds \; + \; \mathcal{O}(\varepsilon^3 |t|) \\
&\quad \stackrel{(41)}{=} \quad \mathrm{i} \mathrm{e}^{-\mathrm{i} H^\varepsilon_{\mathcal{A}} t} \int_0^t \mathrm{e}^{\mathrm{i} H^\varepsilon_{\mathcal{A}} s} \, (A^* H^\varepsilon - H^\varepsilon_{\mathcal{A}} A^*) \, P^\varepsilon \, \chi(H^\varepsilon) \mathrm{e}^{-\mathrm{i} H_\varepsilon s} \, A \, ds \; + \; \mathcal{O}(\varepsilon^3 |t|) \\
&\quad = \quad \mathcal{O}(\varepsilon^3 |t|)
\end{aligned}
$$

due to (43) and $\|\chi(H^\varepsilon)\|_{\mathcal{L}(\overline{\mathcal{H}}, \mathcal{D}(H^\varepsilon))} \lesssim 1$. The latter holds because H^ε is bounded from below and the support of χ is bounded from above, both independent of ε. $\qquad \square$

Proof of Corollary 5:

We will only prove that (42) is a consequence of the other statements. These follow directly from Lemma 2 by making use of the unitarity of M_ρ and D_ε as well as of $D_\varepsilon \langle \nu \rangle D_\varepsilon^* = \langle \nu / \varepsilon \rangle$, when we recall that $P^\varepsilon = M_\rho D_\varepsilon P_\varepsilon D_\varepsilon^* M_\rho^*$ from the proof of Theorem 1.

We prove (42) by induction. For $m = 0$ both statements are clear. Now we assume that it is true for some fixed $m \in \mathbb{N}_0$. Theorem 1 yields that $P^\varepsilon = U^{\varepsilon*} U^\varepsilon$ and $H^\varepsilon_{\mathrm{eff}} = U^\varepsilon H^\varepsilon U^{\varepsilon*}$. On the one hand, this implies

$$
H^{\varepsilon^{m+1}}_{\mathrm{eff}} U^\varepsilon \; = \; H^{\varepsilon^m}_{\mathrm{eff}} U^\varepsilon H^\varepsilon P^\varepsilon .
$$

Then $\|P^\varepsilon\|_{\mathcal{L}(\mathcal{D}(H^{\varepsilon^{m+1}}))} \lesssim 1$ and the induction assumption immediately imply $\|U^\varepsilon\|_{\mathcal{L}(\mathcal{D}(H^{\varepsilon^{m+1}}), \mathcal{D}(H^{\varepsilon^{m+1}}_{\mathrm{eff}}))} \lesssim 1$. On the other hand, we have

$$
\begin{aligned}
H^{\varepsilon^{m+1}} U^{\varepsilon*} \; &= \; H^{\varepsilon^m} P^\varepsilon H^\varepsilon U^{\varepsilon*} + H^{\varepsilon^m} [H^\varepsilon, P^\varepsilon] U^{\varepsilon*} \\
&= \; H^{\varepsilon^m} U^{\varepsilon*} H^\varepsilon_{\mathrm{eff}} + H^{\varepsilon^m} [H^\varepsilon, P^\varepsilon] U^{\varepsilon*} .
\end{aligned}
$$

By the induction assumption and (40) it holds for all ψ that

$$
\begin{aligned}
\|H^{\varepsilon^{m+1}} U^{\varepsilon*} \psi\| \; &\leq \; \|H^{\varepsilon^m} U^{\varepsilon*} H^\varepsilon_{\mathrm{eff}} \psi\| + \|H^{\varepsilon^m} [H^\varepsilon, P^\varepsilon] U^{\varepsilon*} \psi\| \\
&\lesssim \; \|H^{\varepsilon^{m+1}}_{\mathrm{eff}} \psi\| + \|H^\varepsilon_{\mathrm{eff}} \psi\| + \varepsilon \left(\|H^{\varepsilon^{m+1}} U^{\varepsilon*} \psi\| + \|H^{\varepsilon^m} U^{\varepsilon*} \psi\| \right) \\
&\lesssim \; \|H^{\varepsilon^{m+1}}_{\mathrm{eff}} \psi\| + \varepsilon \|H^{\varepsilon^{m+1}} U^{\varepsilon*} \psi\| + \|\psi\| ,
\end{aligned}
$$

where we used that lower powers of a self-adjoint operator are operator-bounded by higher powers. For ε small enough, we can absorb the term with the ε on the left-hand side, which yields $\|U^{\varepsilon*}\|_{\mathcal{L}(D(H^{\varepsilon^{m+1}}_{\mathrm{eff}}), \mathcal{D}(H^{\varepsilon^{m+1}}))} \lesssim 1$. $\qquad \square$

3.3 Derivation of the effective Hamiltonian

The goal of this section is to prove Theorem 2. We first take a closer look at the horizontal connection ∇^{h} (see Definition 1):

Lemma 4 *It holds* $\langle \nabla^{\mathrm{h}}_{\tau}\phi|\psi\rangle_{\mathcal{H}_{\mathrm{f}}} + \langle \phi|\nabla^{\mathrm{h}}_{\tau}\psi\rangle_{\mathcal{H}_{\mathrm{f}}} = \big(\mathrm{d}\langle\phi|\psi\rangle_{\mathcal{H}_{\mathrm{f}}}\big)(\tau)$ *and*

$$\mathrm{R}^{\mathrm{h}}(\tau_1, \tau_2)\psi := \Big(\nabla^{\mathrm{h}}_{\tau_1}\nabla^{\mathrm{h}}_{\tau_2} - \nabla^{\mathrm{h}}_{\tau_2}\nabla^{\mathrm{h}}_{\tau_1} - \nabla^{\mathrm{h}}_{[\tau_1,\tau_2]}\Big)\psi = -\nabla^{\mathrm{v}}_{\mathrm{R}^{\perp}(\tau_1,\tau_2)\nu}\psi, \quad (44)$$

where $\mathrm{R}^{\perp}$ *is the normal curvature mapping (defined in the appendix).*

The proof of this result can be found at the beginning of Section 4.

In order to deduce the formula for the effective Hamiltonian we need that H_{ε} can be expanded with respect to the normal directions when operating on functions that decay fast enough. For this purpose we split up the integral over $N\mathcal{C}$ into an integral 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 e.g. chapter XVI, §4 of [23]).

Lemma 5 *Let* $m \in \mathbb{N}_0$. *If a densely defined operator A satisfies*

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

for every $l \in \mathbb{N}$, *then the operators* $H_{\varepsilon}A, AH_{\varepsilon} \in \mathcal{L}\big(\mathcal{D}(H^{m+1}_{\varepsilon}),\mathcal{H}\big)$ *can be expanded in powers of* ε:

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

where H_0, H_1, H_2 *are the operators associated with*

$$\langle\phi|H_0\psi\rangle_{\mathcal{H}} = \int_{\mathcal{C}}\int_{N_q\mathcal{C}} g(\varepsilon\nabla^{\mathrm{h}}\phi^*, \varepsilon\nabla^{\mathrm{h}}\psi)\, d\nu\, d\mu + \langle\phi|H_{\mathrm{f}}\psi\rangle_{\mathcal{H}}, \quad (45)$$

$$\langle\phi|H_1\psi\rangle_{\mathcal{H}} = \int_{\mathcal{C}}\int_{N_q\mathcal{C}} 2\,\mathrm{II}_{\nu}\big(\varepsilon\nabla^{\mathrm{h}}\phi^*, \varepsilon\nabla^{\mathrm{h}}\psi\big) + \phi^*\big(\nabla^{\mathrm{v}}_{\nu}W\big)\psi\, d\nu\, d\mu,$$

$$\begin{aligned}
\langle\phi|H_2\psi\rangle_{\mathcal{H}} = \int_{\mathcal{C}}\int_{N_q\mathcal{C}} & 3\,g\big(\mathcal{W}_{\nu}\,\varepsilon\nabla^{\mathrm{h}}\phi^*, \mathcal{W}_{\nu}\,\varepsilon\nabla^{\mathrm{h}}\psi\big) + \mathcal{R}\big(\varepsilon\nabla^{\mathrm{h}}\phi^*, \nu, \varepsilon\nabla^{\mathrm{h}}\psi, \nu\big) \\
& + \tfrac{2}{3}\mathcal{R}\big(\varepsilon\nabla^{\mathrm{h}}\phi^*, \nu, \nabla^{\mathrm{v}}\psi, \nu\big) + \tfrac{2}{3}\mathcal{R}\big(\nabla^{\mathrm{v}}\phi^*, \nu, \varepsilon\nabla^{\mathrm{h}}\psi, \nu\big) \\
& + \tfrac{1}{3}\mathcal{R}\big(\nabla^{\mathrm{v}}\phi^*, \nu, \nabla^{\mathrm{v}}\psi, \nu\big) + \phi^*\big(\tfrac{1}{2}\nabla^{\mathrm{v}}_{\nu,\nu}W + V_{\mathrm{geom}}\big)\psi\, d\nu\, d\mu,
\end{aligned}$$

where II *is the second fundamental form,* $\mathcal{W}$ *is the Weingarten mapping, and* $\mathcal{R}$ *is the Riemann tensor (see the appendix for the definitions). Furthermore, for* $l \in \{0, 1, 2\}$

$$\|H_l A\|_{\mathcal{L}(\mathcal{D}(H^{m+1}_{\varepsilon}),\mathcal{H})} \lesssim 1, \quad \|AH_l\|_{\mathcal{L}(\mathcal{D}(H^{m+1}_{\varepsilon}),\mathcal{H})} \lesssim 1. \quad (46)$$

This will be proved in Section 4.2. Definition 3, Lemma 2, and the following lemma imply that Lemma 5 can be applied to the 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_f, and $\tilde{U}_\varepsilon$ (see Remark 1 and Lemma 2):

Lemma 6 *It holds $E_f \in C_b^\infty(\mathcal{C})$, as well as:*

i) $\forall\, l, j \in \mathbb{N}_0 :\ \| \langle \nu \rangle^l P_0 \langle \nu \rangle^j \|_{\mathcal{L}(\mathcal{D}(H_\varepsilon))} \lesssim 1\,,\ \| [-\varepsilon^2 \Delta_h, P_0] \|_{\mathcal{L}(\mathcal{D}(H_\varepsilon), \mathcal{H})} \lesssim \varepsilon.$

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) $\| P_0 U_1^\varepsilon \langle \nu \rangle^l \|_{\mathcal{L}(\mathcal{D}(H_\varepsilon^m))} \lesssim 1$ *for all $l \in \mathbb{N}_0$ and $m \in \{0, 1\}$.*

iv) *For $B_\varepsilon := P_0 \tilde{U}_\varepsilon \chi(H_\varepsilon)$ and all $u \in \{1, (U_1^\varepsilon)^*, (U_2^\varepsilon)^*\}$ it holds*

$$\big\| \, [-\varepsilon^2 \Delta_h + E_f, u P_0] \, B_\varepsilon \, \big\|_{\mathcal{L}(\mathcal{H})} \;=\; \mathcal{O}(\varepsilon). \tag{47}$$

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

$$\big\| U_1^{\varepsilon *} B_\varepsilon \,+\, R_{H_f}(E_f)\,([-\varepsilon \Delta_h, P_0] + H_1) P_0 B_\varepsilon \big\|_{\mathcal{L}(\mathcal{H}, \mathcal{D}(H_\varepsilon))} = \mathcal{O}(\varepsilon) \tag{48}$$

vi) *If $\varphi_f \in C_b^\infty(\mathcal{C}, \mathcal{H}_f)$, it holds*

$$\| U_0 \|_{\mathcal{L}(\mathcal{D}(H_\varepsilon), \mathcal{D}(-\varepsilon^2 \Delta_{\mathcal{C}} + E_f))} \lesssim 1, \quad \| U_0^* \|_{\mathcal{L}(\mathcal{D}(-\varepsilon^2 \Delta_{\mathcal{C}} + E_f), \mathcal{D}(H_\varepsilon))} \lesssim 1,$$

and there is $\lambda_0 \gtrsim 1$ with $\sup_q \| e^{\lambda_0 \langle \nu \rangle} \varphi_f(q) \|_{\mathcal{H}_f(q)} \lesssim 1$ and

$$\sup_{q \in \mathcal{C}} \| e^{\lambda_0 \langle \nu \rangle} \nabla^v_{\nu_1, \ldots, \nu_l} \nabla^h_{\tau_1, \ldots, \tau_m} \varphi_f(q) \|_{\mathcal{H}_f(q)} \lesssim 1$$

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

The proof of this lemma can be found in Section 4.3. Since U_2^ε does only effect $P_\varepsilon \mathcal{H}$ but not the effective Hamiltonian, we have not stated its particular form here, as we did for U_1^ε in v). To calculate the effective Hamiltonian we also need the following estimates for energy cutoffs.

Lemma 7 *Assume that $\big(H, \mathcal{D}(H)\big)$ is self-adjoint on some Hilbert space $\mathcal{H}$. Let $\chi_1 \in C_0^\infty(\mathbb{R})$ and $\chi_2 : \mathbb{R} \to \mathbb{R}$ be a bounded Borel function.*

a) Let $A \in \mathcal{L}(\mathcal{H})$. If $\big\| [H, A] \chi_2(H) \big\|_{\mathcal{L}(\mathcal{D}(H^l), \mathcal{D}(H^{m-1}))} \leq \delta$ for some $l, m \in \mathbb{N}$, then there is $C < \infty$ depending only on χ_1 such that

$$\big\| [\chi_1(H), A] \chi_2(H) \big\|_{\mathcal{L}(\mathcal{D}(H^{l-1}), \mathcal{D}(H^m))} \leq C \delta.$$

b) Let $\left(\tilde{H}, \mathcal{D}(\tilde{H})\right)$ *be also self-adjoint on* $\mathcal{H}$. *If there are* $l, m \in \mathbb{N}$ *with* $\left\|(H - \tilde{H})\chi_2(\tilde{H})\right\|_{\mathcal{L}(\mathcal{D}(\tilde{H}^l), \mathcal{D}(H^{m-1}))} \leq \delta$, *then there is* $C < \infty$ *depending only on* χ_1 *such that*

$$\left\|(\chi_1(H) - \chi_1(\tilde{H}))\chi_2(\tilde{H})\right\|_{\mathcal{L}(\mathcal{D}(\tilde{H}^{l-1}), \mathcal{D}(H^m))} \leq C\delta.$$

c) Let $\tilde{\mathcal{H}}$ *be another Hilbert space and* $B \in \mathcal{L}(\mathcal{H}, \tilde{\mathcal{H}})$ *such that* $BB^* = 1$ *and* $\left(\tilde{H} := BHB^*, \mathcal{D}(\tilde{H})\right)$ *is self-adjoint on* $\tilde{\mathcal{H}}$. *Assume that there is* $m \in \mathbb{N}$ *such that* $B \in \mathcal{L}\left(\mathcal{D}(H^l), \mathcal{D}(\tilde{H}^l)\right)$ *and* $B^* \in \mathcal{L}\left(\mathcal{D}(\tilde{H}^l), \mathcal{D}(H^l)\right)$ *for all* $l \leq m$.

  i) If $\chi_2 \in C_0^\infty(\mathbb{R})$ *and* $\left\|[H, B^*B]\chi_2(H)\right\|_{\mathcal{L}(\mathcal{H}, \mathcal{D}(H^m))} \leq \delta$, *then there is* $C < \infty$ *depending only on* χ_1, χ_2, $\|B\|_{\mathcal{L}(\mathcal{D}(H^l), \mathcal{D}(\tilde{H}^l))}$, $\|B^*\|_{\mathcal{L}(\mathcal{D}(\tilde{H}^l), \mathcal{D}(H^l))}$ *for* $l \leq m$ *such that*

$$\left\|(\chi_1(\tilde{H}) - B\chi_1(H)B^*)B\chi_2^2(H)\right\|_{\mathcal{L}(\mathcal{H}, \mathcal{D}(\tilde{H}^m))} \leq C\delta.$$

  ii) If $\left\|[H, B^*B]\right\|_{\mathcal{L}(\mathcal{D}(H^m), \mathcal{D}(H^{m-1}))} \leq \delta$, *then there is* $C < \infty$ *depending only on* χ_1, $\|B\|_{\mathcal{L}(\mathcal{D}(H^l), \mathcal{D}(\tilde{H}^l))}$, *and* $\|B^*\|_{\mathcal{L}(\mathcal{D}(\tilde{H}^l), \mathcal{D}(H^l))}$ *for* $l \leq m$ *such that*

$$\left\|\chi_1(\tilde{H}) - B\chi_1(H)B^*\right\|_{\mathcal{L}(\mathcal{D}(\tilde{H}^{m-1}), \mathcal{D}(\tilde{H}^m))} \leq C\delta^2.$$

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 in a) and b) need not be compact, in particular $\chi_2 \equiv 1$ is allowed there. Now we are ready to derive the theorem about the form of the effective Hamiltonian. We deduce its corollary concerning the unitary groups before. Lemma 7 will be proved afterwards.

PROOF OF COROLLARY 2 (SECTION 2.2):
In order to check that

$$\left\|\left(e^{-iH^\varepsilon t} - U_0^{\varepsilon*}e^{-iH_{\text{eff}}^{(2)}t}U_0^\varepsilon\right)U_0^{\varepsilon*}\chi(H_{\text{eff}}^{(2)})U_0^\varepsilon\right\|_{\mathcal{L}(\overline{\mathcal{H}})} \lesssim \varepsilon(1 + \varepsilon^2|t|), \quad (49)$$

with $U_0^\varepsilon = U_0 D_\varepsilon^*$, indeed, follows from Theorem 1 and Theorem 2 we start by verifying that $\|U^\varepsilon - U_0^\varepsilon\|_{\mathcal{L}(\overline{\mathcal{H}}, \mathcal{H}_{\text{eff}})} = \mathcal{O}(\varepsilon)$.

We recall that we defined $\tilde{\rho} := \frac{d\mu}{d\mu_{\text{eff}}^\varepsilon}$ as well as $U^\varepsilon := M_{\tilde{\rho}}^* U_0 \tilde{U}_\varepsilon D_\varepsilon^* M_\rho^*$ in the proof of Theorem 1. Since $d\mu_{\text{eff}}^\varepsilon$ is the volume measure associated to $g_{\text{eff}}^\varepsilon$, which is given by the expression in Theorem 2, we have $\|\tilde{\rho} - 1\|_\infty = \mathcal{O}(\varepsilon)$ and thus $\|M_{\tilde{\rho}} - 1\|_{\mathcal{L}(L^2(\mathcal{C}, d\mu))} = \mathcal{O}(\varepsilon)$. Using in addition that $\|\tilde{U}_\varepsilon - 1\|_{\mathcal{L}(\mathcal{H})} = \mathcal{O}(\varepsilon)$

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by Lemma 6 and $M_{\tilde\rho}^* M_{\tilde\rho} = 1$ we obtain that

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

because $U_0 = U_0 P_0$ and the projector P_0 associated to the constraint energy band E_{f} satisfies $\|P_0\langle\nu\rangle\|_{\mathcal{L}(\mathcal{H})} \lesssim 1$ by assumption (see Definition 3). In view of (19), a first order Taylor expansion of ρ in normal directions yields that $D_\varepsilon^*(M_\rho^* - 1)$ is globally bounded by a constant times $\varepsilon\langle\nu\rangle$. Hence, we end up with $\|U^\varepsilon - U_0^\varepsilon\|_{\mathcal{L}(\overline{\mathcal{H}}, \mathcal{H}_{\mathrm{eff}})} = \mathcal{O}(\varepsilon)$ and may thus replace U_0^ε by U^ε in (49).

Now let $\chi : \mathbb{R} \to [-1, 1]$ be a Borel function with $\mathrm{supp}\,\chi \subset (-\infty, E]$. Using the triangle inequality and $U^\varepsilon U^{\varepsilon*} = 1$ we see that

$$
\begin{aligned}
\left\| \left(\mathrm{e}^{-\mathrm{i}H^\varepsilon t} - U^{\varepsilon*} \mathrm{e}^{-\mathrm{i}H_{\mathrm{eff}}^{(2)} t} U^\varepsilon \right) U^{\varepsilon*} \chi(H_{\mathrm{eff}}^{(2)}) U^\varepsilon \right\|_{\mathcal{L}(\overline{\mathcal{H}})} & \\
\leq \left\| \left(\mathrm{e}^{-\mathrm{i}H^\varepsilon t} - U^{\varepsilon*} \mathrm{e}^{-\mathrm{i}H_{\mathrm{eff}}^\varepsilon t} U^\varepsilon \right) U^{\varepsilon*} \chi(H_{\mathrm{eff}}^{(2)}) U^\varepsilon \right\|_{\mathcal{L}(\overline{\mathcal{H}})} & \\
+ \left\| U^{\varepsilon*} \left(\mathrm{e}^{-\mathrm{i}H_{\mathrm{eff}}^\varepsilon t} - \mathrm{e}^{-\mathrm{i}H_{\mathrm{eff}}^{(2)} t} \right) \chi(H_{\mathrm{eff}}^{(2)}) U^\varepsilon \right\|_{\mathcal{L}(\overline{\mathcal{H}})}. & \quad (50)
\end{aligned}
$$

The second term is of order $\varepsilon^3 |t|$ because

$$
\begin{aligned}
&\left(\mathrm{e}^{-\mathrm{i}H_{\mathrm{eff}}^\varepsilon t} - \mathrm{e}^{-\mathrm{i}H_{\mathrm{eff}}^{(2)} t} \right) \chi(H_{\mathrm{eff}}^{(2)}) \\
&= \mathrm{i}\mathrm{e}^{-\mathrm{i}H_{\mathrm{eff}}^\varepsilon t} \int_0^t \mathrm{e}^{\mathrm{i}H_{\mathrm{eff}}^\varepsilon s} \left(H_{\mathrm{eff}}^{(2)} - H_{\mathrm{eff}}^\varepsilon \right) \mathrm{e}^{\mathrm{i}H_{\mathrm{eff}}^{(2)} s} \chi(H_{\mathrm{eff}}^{(2)}) \, ds \\
&= \mathrm{i}\mathrm{e}^{-\mathrm{i}H_{\mathrm{eff}}^\varepsilon t} \int_0^t \mathrm{e}^{\mathrm{i}H_{\mathrm{eff}}^\varepsilon s} \left(H_{\mathrm{eff}}^{(2)} - H_{\mathrm{eff}}^\varepsilon \right) \chi(H_{\mathrm{eff}}^{(2)}) \mathrm{e}^{\mathrm{i}H_{\mathrm{eff}}^{(2)} s} \, ds = \mathcal{O}(\varepsilon^3 |t|)
\end{aligned}
$$

by Theorem 2. Let $\tilde\chi \in C_0^\infty(\mathbb{R})$ with $\mathrm{supp}\,\tilde\chi|_{[\inf \sigma(H_{\mathrm{eff}}^{(2)}), E]} \equiv 1$. By Theorem 2 and Lemma 7 b) we have

$$
\begin{aligned}
U^{\varepsilon*} \chi(H_{\mathrm{eff}}^{(2)}) &= U^{\varepsilon*} \tilde\chi(H_{\mathrm{eff}}^{(2)}) \chi(H_{\mathrm{eff}}^{(2)}) \\
&= U^{\varepsilon*} \tilde\chi(H_{\mathrm{eff}}^\varepsilon) \chi(H_{\mathrm{eff}}^{(2)}) + \mathcal{O}(\varepsilon^3).
\end{aligned}
$$

We recall from Theorem 1 that $H_{\mathrm{eff}}^\varepsilon = U^\varepsilon H^\varepsilon U^{\varepsilon*}$ and $P^\varepsilon = U^{\varepsilon*} U^\varepsilon$. In view of Corollary 5, U^ε satisfies the assumptions on B in Lemma 7 c) ii) with $\delta = \varepsilon$.

Therefore

$$
\begin{aligned}
U^{\varepsilon*}\chi(H^{(2)}_{\text{eff}}) \;&=\; U^{\varepsilon*}\tilde{\chi}(U^{\varepsilon}H^{\varepsilon}U^{\varepsilon*})\chi(H^{(2)}_{\text{eff}}) \;+\; \mathcal{O}(\varepsilon^3) \\
&=\; U^{\varepsilon*}U^{\varepsilon}\tilde{\chi}(H^{\varepsilon})U^{\varepsilon*}\chi(H^{(2)}_{\text{eff}}) \;+\; \mathcal{O}(\varepsilon^2) \\
&=\; P^{\varepsilon}\tilde{\chi}(H^{\varepsilon})U^{\varepsilon*}\chi(H^{(2)}_{\text{eff}}) \;+\; \mathcal{O}(\varepsilon^2).
\end{aligned}
$$

After plugging this into the first term in (50) we may apply Theorem 1 to it. This yields the claim. $\qquad\square$

Proof of Theorem 2 (Section 2.2):
We recall that we defined $U_{\varepsilon} := U_0\tilde{U}_{\varepsilon}$, $U^{\varepsilon} := M^*_{\tilde{\rho}}U_{\varepsilon}D^*_{\varepsilon}M^*_{\rho}$, $P^{\varepsilon} := U^{\varepsilon*}U^{\varepsilon}$, and $H^{\varepsilon}_{\text{eff}} := U^{\varepsilon}H^{\varepsilon}U^{\varepsilon*}$ in the proof of Theorem 1, which implied $P_{\varepsilon} = U^*_{\varepsilon}U_{\varepsilon}$. Let $\chi : \mathbb{R} \to [-1, 1]$ be a Borel function with $\operatorname{supp}\chi \subset (-\infty, E]$.
Furthermore, we recall that $\mathcal{D}(A)$ always denotes the maximal domain of an operator A (i.e. all ψ with $\|A\psi\| + \|\psi\| < \infty$) equipped with the graph norm. A differential operator A of order m will be called elliptic on $(\mathcal{C}, g)$, if it satisfies $\big[\ldots[\underbrace{A, f]\ldots, f}_{m-times}\big] \geq c|\mathrm{d}f|^m_g$ for some $c > 0$ and any f.

We set $H^{(0)}_{\text{eff}} := -\varepsilon^2\Delta_{\mathcal{C}} + E_{\text{f}}$ with $\Delta_{\mathcal{C}}$ the Laplace-Beltrami operator on $(\mathcal{C}, g)$. Since $E_{\text{f}} \in C^{\infty}_{\text{b}}(\mathcal{C})$ due to Lemma 6, all powers of $H^{(0)}_{\text{eff}}$ are obviously elliptic operators of class $C^{\infty}_{\text{b}}(\mathcal{C})$ on $\mathcal{H}_{\text{eff}}$. This implies that $\big(H^{(0)}_{\text{eff}}, \mathcal{D}(H^{(0)}_{\text{eff}})\big)$ is self-adjoint on $\mathcal{H}_{\text{eff}}$ because $\mathcal{C}$ is of bounded geometry (see Section 1.4. of [40]; in particular, this entails that $\mathcal{D}(H^{(0)}_{\text{eff}})$ is the Sobolev space $W^{2,2}(\mathcal{C})$, but equipped with an ε-dependent norm). Let $E_{-} := \min\{\inf\sigma(H^{\varepsilon}), \inf\sigma(H^{(0)}_{\text{eff}})\}$ and $\tilde{\chi}, \tilde{\tilde{\chi}} \in C^{\infty}_0(\mathbb{R})$ with $\tilde{\chi}|_{[E_-, E]} \equiv 1$ and $\tilde{\tilde{\chi}}|_{\operatorname{supp}\tilde{\chi}} \equiv 1$. Then we define $H^{(2)}_{\text{eff}}$ for $\phi, \psi \in \mathcal{D}(H^{(0)}_{\text{eff}})$ by

$$
\begin{aligned}
\langle\,\phi\,|\,H^{(2)}_{\text{eff}}\,\psi\,\rangle \;:=\; \int_{\mathcal{C}} \Big(&g^{\varepsilon}_{\text{eff}}\big((p^{\varepsilon}_{\text{eff}}\phi)^*, p^{\varepsilon}_{\text{eff}}\psi\big) \;+\; \phi^*\big(E_{\text{f}} + \varepsilon\,\langle\varphi_{\text{f}}|(\nabla^{\text{v}}W)\varphi_{\text{f}}\rangle_{\mathcal{H}_{\text{f}}}\big)\,\psi \\
&+ \phi^*\varepsilon^2\,W^{(2)}\,\psi \;-\; \varepsilon^2\,\mathcal{M}\big(\Phi^*(\phi), \Phi(\tilde{\tilde{\chi}}(H^{(0)}_{\text{eff}})\psi)\big) \qquad (51) \\
&- \varepsilon^2\,\mathcal{M}\big(\Phi^*(\tilde{\tilde{\chi}}(H^{(0)}_{\text{eff}})\phi), \Phi(\psi - \tilde{\tilde{\chi}}(H^{(0)}_{\text{eff}})\psi)\big)\Big)\,d\mu^{\varepsilon}_{\text{eff}}
\end{aligned}
$$

where $\Phi(\psi) := \Psi(\varepsilon\nabla p^{\varepsilon}_{\text{eff}}\psi, p^{\varepsilon}_{\text{eff}}\psi, \psi)$ and all the other objects are defined by the expressions in Theorem 2. Because of $\tilde{\tilde{\chi}}(H^{(0)}_{\text{eff}})\chi(H^{(0)}_{\text{eff}}) = \chi(H^{(0)}_{\text{eff}})$ this definition immediately implies that $H^{(2)}_{\text{eff}}$ operates on ψ with $\psi = \chi(H^{(0)}_{\text{eff}})\psi$ as stated in the theorem. The rest of the proof will be devided into several steps.

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Step 1: $\big(H_{\mathrm{eff}}^{(2)}, \mathcal{D}(H_{\mathrm{eff}}^{(0)})\big)$ *is self-adjoint on* $\mathcal{H}_{\mathrm{eff}}$ *and*

$$\|H_{\mathrm{eff}}^{(2)} - H_{\mathrm{eff}}^{(0)}\|_{\mathcal{L}(\mathcal{D}(H_{\mathrm{eff}}^{(0)}), \mathcal{H}_{\mathrm{eff}})} = \mathcal{O}(\varepsilon).$$

It easy to verify that $H_{\mathrm{eff}}^{(2)}$ is symmetric. Then it suffices to prove the stated estimate because by the Kato-Rellich theorem (see e.g. [36]) the estimate implies that $\big((H_{\mathrm{eff}}^{(2)}, \mathcal{D}(H_{\mathrm{eff}}^{(0)})\big)$ is self-adjoint on $\mathcal{H}_{\mathrm{eff}}$ for ε small enough.

Since $\mathcal{C}$ is of bounded geometry, maximal regularity estimates hold true there (see Appendix 1 of [40]), in particular, differential operators of order $m \in \mathbb{N}$ with coefficients in $C_{\mathrm{b}}^{\infty}(\mathcal{C})$ are bounded by elliptic operators of same order and class.

The operator M associated to $\int_{\mathcal{C}} \mathcal{M}\big(\Phi(\phi), \Phi(\psi)\big) d\mu_{\mathrm{eff}}^{\varepsilon}$ is a fourth order differential operator which, in view of Lemma 6 vi), has coefficients in $C_{\mathrm{b}}^{\infty}(\mathcal{C})$. Hence, it is bounded by $(H_{\mathrm{eff}}^{(0)})^2$ with a constant independent of ε because all derivatives carry an ε. We notice that $\|\tilde{\tilde{\chi}}(H_{\varepsilon})\|_{\mathcal{L}(\mathcal{H}, \mathcal{D}(H_{\mathrm{eff}}^{(0)m}))} \lesssim 1$ for all $m \in \mathbb{N}_0$ because the support of $\tilde{\tilde{\chi}}$ is bounded independently of ε. Thus we obtain that $M\tilde{\chi}(H_{\mathrm{eff}}^{(0)})$ is bounded. The same is true for $\tilde{\chi}(H_{\mathrm{eff}}^{(0)})M\big(1 - \tilde{\chi}(H_{\mathrm{eff}}^{(0)})\big)$ because it is operator-bounded by the adjoint of $M\tilde{\chi}(H_{\mathrm{eff}}^{(0)})$. Therefore the $\mathcal{M}$-terms in (51) correspond to bounded operators! All the other terms are associated to differential operators of second order whose coeffcients are in $C_{\mathrm{b}}^{\infty}(\mathcal{C})$ by Lemma 6 vi) and whose derivatives carry at least one ε each. Therefore they are bounded by the elliptic $H_{\mathrm{eff}}^{(0)}$.

So we obtain that $\|H_{\mathrm{eff}}^{(2)} - H_{\mathrm{eff}}^{(0)}\|_{\mathcal{L}(\mathcal{D}(H_{\mathrm{eff}}^{(0)}), \mathcal{H}_{\mathrm{eff}})} = \mathcal{O}(\varepsilon)$ by observing that the leading order of $H_{\mathrm{eff}}^{(2)}$ is indeed $H_{\mathrm{eff}}^{(0)}$.

Step 2: $\mathcal{D}(H_{\mathrm{eff}}^{\varepsilon}) = \mathcal{D}(H_{\mathrm{eff}}^{(0)})$ *and* $\|H_{\mathrm{eff}}^{\varepsilon} - H_{\mathrm{eff}}^{(0)}\|_{\mathcal{L}(\mathcal{D}(H_{\mathrm{eff}}^{\varepsilon}), \mathcal{H}_{\mathrm{eff}})} = \mathcal{O}(\varepsilon).$

Since $\|\tilde{U}_{\varepsilon}\|_{\mathcal{L}(\mathcal{D}(H_{\varepsilon}))} \lesssim 1$ and $\|U_0\|_{\mathcal{L}(\mathcal{D}(H_{\varepsilon}), \mathcal{D}(H_{\mathrm{eff}}^{(0)}))} \lesssim 1$ by Lemma 6, it also holds $\|U^{\varepsilon}\|_{\mathcal{L}(\mathcal{D}(H^{\varepsilon}), \mathcal{D}(H_{\mathrm{eff}}^{(0)}))} \lesssim 1$. Using, in addition, that $\|U^{\varepsilon*}\|_{\mathcal{L}(\mathcal{D}(H^{\varepsilon}), \mathcal{D}(H_{\mathrm{eff}}^{\varepsilon}))} \lesssim 1$ due to Corollary 5 and $U^{\varepsilon}U^{\varepsilon*} = 1$ we conclude that for all $\psi \in \mathcal{D}(H_{\mathrm{eff}}^{\varepsilon})$

$$\|\psi\|_{\mathcal{D}(H_{\mathrm{eff}}^{(0)})} = \|U^{\varepsilon}U^{\varepsilon*}\psi\|_{\mathcal{D}(H_{\mathrm{eff}}^{(0)})} \lesssim \|U^{\varepsilon*}\psi\|_{\mathcal{D}(H^{\varepsilon})} \lesssim \|\psi\|_{\mathcal{D}(H_{\mathrm{eff}}^{\varepsilon})}.$$

On the other hand, Lemma 6 and Corollary 5 imply via the analogous arguments that for all $\psi \in \mathcal{D}(H_{\mathrm{eff}}^{(0)})$

$$\|\psi\|_{\mathcal{D}(H_{\mathrm{eff}}^{\varepsilon})} = \|U^{\varepsilon}U^{\varepsilon*}\psi\|_{\mathcal{D}(H_{\mathrm{eff}}^{\varepsilon})} \lesssim \|U^{\varepsilon*}\psi\|_{\mathcal{D}(H^{\varepsilon})} \lesssim \|\psi\|_{\mathcal{D}(H_{\mathrm{eff}}^{(0)})}.$$

Hence, $\mathcal{D}(H_{\mathrm{eff}}^{\varepsilon}) = \mathcal{D}(H_{\mathrm{eff}}^{(0)})$.

Using $H_{\mathrm{eff}}^{\varepsilon} = U^{\varepsilon} H^{\varepsilon} U^{\varepsilon*} = U^{\varepsilon} P^{\varepsilon} H^{\varepsilon} P^{\varepsilon} U^{\varepsilon*}$ and again Corollary 5 we get

$$
\begin{aligned}
\|H_{\mathrm{eff}}^{\varepsilon} &- H_{\mathrm{eff}}^{(0)}\|_{\mathcal{L}(\mathcal{D}(H_{\mathrm{eff}}^{\varepsilon}),\mathcal{H}_{\mathrm{eff}})}\\
&= \|U^{\varepsilon}(P^{\varepsilon} H^{\varepsilon} P^{\varepsilon} - U^{\varepsilon*} H_{\mathrm{eff}}^{(0)} U^{\varepsilon}) U^{\varepsilon*}\|_{\mathcal{L}(\mathcal{D}(H_{\mathrm{eff}}^{\varepsilon}),\mathcal{H}_{\mathrm{eff}})}\\
&\lesssim \|P^{\varepsilon} H^{\varepsilon} P^{\varepsilon} - U^{\varepsilon*} H_{\mathrm{eff}}^{(0)} U^{\varepsilon}\|_{\mathcal{L}(\mathcal{D}(H^{\varepsilon}),\overline{\mathcal{H}})}\\
&= \|P_{\varepsilon} H_{\varepsilon} P_{\varepsilon} - U_{\varepsilon}^{*} M_{\tilde{\rho}} H_{\mathrm{eff}}^{(0)} M_{\tilde{\rho}}^{*} U_{\varepsilon}\|_{\mathcal{L}(\mathcal{D}(H_{\varepsilon}),\mathcal{H})}\\
&= \|P_{0} H_{\varepsilon} P_{0} - U_{0}^{*} M_{\tilde{\rho}} H_{\mathrm{eff}}^{(0)} M_{\tilde{\rho}}^{*} U_{0}\|_{\mathcal{L}(\mathcal{D}(H_{\varepsilon}),\mathcal{H})} + \mathcal{O}(\varepsilon)
\end{aligned}
$$

because $P_{\varepsilon} = U_{\varepsilon}^{*} U_{\varepsilon}$, $U_{\varepsilon} = U_{0} \tilde{U}_{\varepsilon}$, and by Lemma 6 ii) it holds $\tilde{U}_{\varepsilon} - 1 = \mathcal{O}(\varepsilon)$ both in $\mathcal{L}(\mathcal{H})$ and in $\mathcal{L}(\mathcal{D}(H_{\varepsilon}))$. Lemma 5 implies that $P_{0}(H_{\varepsilon} - H_{0})P_{0} = \mathcal{O}(\varepsilon)$ in $\mathcal{L}(\mathcal{D}(H_{\varepsilon}),\mathcal{H})$. Hence,

$$
\begin{aligned}
\|H_{\mathrm{eff}}^{\varepsilon} &- H_{\mathrm{eff}}^{(0)}\|_{\mathcal{L}(\mathcal{D}(H_{\mathrm{eff}}^{\varepsilon}),\mathcal{H}_{\mathrm{eff}})}\\
&= \|P_{0} H_{0} P_{0} - U_{0}^{*} M_{\tilde{\rho}} H_{\mathrm{eff}}^{(0)} M_{\tilde{\rho}}^{*} U_{0}\|_{\mathcal{L}(\mathcal{D}(H_{\varepsilon}),\mathcal{H})} + \mathcal{O}(\varepsilon)\\
&\lesssim \|U_{0} H_{0} U_{0}^{*} - M_{\tilde{\rho}} H_{\mathrm{eff}}^{(0)} M_{\tilde{\rho}}^{*}\|_{\mathcal{L}(\mathcal{D}(H_{\mathrm{eff}}^{(0)}),L^{2}(\mathcal{C},d\mu))} + \mathcal{O}(\varepsilon), \qquad (52)
\end{aligned}
$$

where in the last step we used $P_{0} = U_{0}^{*} U_{0}$ and $\|U_{0}\|_{\mathcal{L}(\mathcal{D}(H_{\varepsilon}),\mathcal{D}(H_{\mathrm{eff}}^{(0)}))} \lesssim 1$ due to Lemma 6 vi). It holds $U_{0}\psi = \varphi_{\mathrm{f}}\psi$ by definiton of U_{0} and $H_{0} = -\Delta_{\mathrm{h}} + H_{\mathrm{f}}$ by Lemma 5. In view of Definition 1, we have

$$
\begin{aligned}
\varepsilon \nabla^{\mathrm{h}} \psi \, \varphi_{\mathrm{f}} &= \varphi_{\mathrm{f}} \, \varepsilon \mathrm{d}\psi + \psi \, \varepsilon \nabla^{\mathrm{h}} \varphi_{\mathrm{f}}, \qquad\qquad\qquad (53)\\
\varepsilon^{2} \Delta_{\mathrm{h}} \psi \, \varphi_{\mathrm{f}} &= \varphi_{\mathrm{f}} \, \varepsilon^{2} \Delta_{\mathcal{C}} \psi + 2g(\varepsilon \mathrm{d}\psi, \varepsilon \nabla^{\mathrm{h}} \varphi_{\mathrm{f}}) + \psi \, \varepsilon^{2} \Delta_{\mathrm{h}} \varphi_{\mathrm{f}},
\end{aligned}
$$

where d is the exterior derivative on $\mathcal{C}$. We note that $\sup_{q} \|\varepsilon \nabla^{\mathrm{h}} \varphi_{\mathrm{f}}\|_{\mathcal{H}_{\mathrm{f}}(q)}$ and $\sup_{q} \|\varepsilon^{2} \Delta_{\mathrm{h}} \varphi_{\mathrm{f}}\|_{\mathcal{H}_{\mathrm{f}}(q)}$ are of order ε and ε^{2} respectively by Lemma 6. Therefore

$$
\begin{aligned}
U_{0} H_{0} U_{0}^{*} \psi = U_{0}(-\varepsilon^{2} \Delta_{\mathrm{h}} + H_{\mathrm{f}}) U_{0}^{*} \psi &= \langle \varphi_{\mathrm{f}} | (-\varepsilon^{2} \Delta_{\mathrm{h}} + E_{\mathrm{f}}) \varphi_{\mathrm{f}} \psi \rangle_{\mathcal{H}_{\mathrm{f}}}\\
&= H_{\mathrm{eff}}^{(0)} \psi + \mathcal{O}(\varepsilon). \qquad (54)
\end{aligned}
$$

We recall that $\tilde{\rho} = d\mu_{\mathrm{eff}}^{\varepsilon}/d\mu$ with $d\mu_{\mathrm{eff}}^{\varepsilon}$ the volume measure associated with $g_{\mathrm{eff}}^{\varepsilon}$. Since $d\mu$ and $d\mu_{\mathrm{eff}}^{\varepsilon}$ coincide at leading order and $\tilde{\rho} \in C_{\mathrm{b}}^{\infty}(\mathcal{C},g)$ by Lemma 6 vi), we have $\|\tilde{\rho} - 1\|_{C^{2}(\mathcal{C},g)} = \mathcal{O}(\varepsilon)$ and thus $\|M_{\tilde{\rho}} - 1\|_{\mathcal{L}(\mathcal{D}(H_{\mathrm{eff}}^{(0)}))} = \mathcal{O}(\varepsilon)$. So we obtain that $\|M_{\tilde{\rho}} H_{\mathrm{eff}}^{(0)} M_{\tilde{\rho}}^{*} - H_{\mathrm{eff}}^{(0)}\|_{\mathcal{L}(\mathcal{D}(H_{\mathrm{eff}}^{(0)}),L^{2}(\mathcal{C},d\mu))} = \mathcal{O}(\varepsilon)$. Together with (52) and (54) this yields $\|H_{\mathrm{eff}}^{\varepsilon} - H_{\mathrm{eff}}^{(0)}\|_{\mathcal{L}(\mathcal{D}(H_{\mathrm{eff}}^{\varepsilon}),\mathcal{H}_{\mathrm{eff}})} = \mathcal{O}(\varepsilon)$.

Step 3: It holds $\|(H_{\mathrm{eff}}^{\varepsilon} - H_{\mathrm{eff}}^{(2)}) U^{\varepsilon} \chi(H^{\varepsilon}) U^{\varepsilon*}\|_{\mathcal{L}(\mathcal{H}_{\mathrm{eff}})} = \mathcal{O}(\varepsilon^{3})$.

This step contains the central order-by-order calculation of $H_{\mathrm{eff}}^{\varepsilon}$ and is therefore by far the longest one. For any ψ we set $\tilde{\psi} := M_{\tilde{\rho}}\psi$, $\psi^{\chi} := U^{\varepsilon} \chi(H^{\varepsilon}) U^{\varepsilon*} \psi$,

and $\tilde{\psi}_\chi := U_\varepsilon \chi(H_\varepsilon) U_\varepsilon^* \tilde{\psi}$. Of course, we have $\|\tilde{\psi}\|_{L^2(\mathcal{C}, d\mu)} = \|\psi\|_{\mathcal{H}_{\text{eff}}}$ and $\|\tilde{\psi}_\chi\|_{L^2(\mathcal{C}, d\mu)} \leq \|\tilde{\psi}\|_{L^2(\mathcal{C}, d\mu)}$ for all $\psi \in \mathcal{H}_{\text{eff}}$.

We first explain why the cut off in the definition of $H_{\text{eff}}^{(2)}$ does not matter here. We note that P^ε and U^ε satisfy the assumption on A and B in Lemma 7 a) and c) ii) with $\delta = \varepsilon$ by Corollary 5. In addition, $H_{\text{eff}}^{(0)}$ and $H_{\text{eff}}^\varepsilon$ satisfy the assumption of Lemma 7 b) with the same δ by Step 2. Therefore

$$
\begin{aligned}
\tilde{\tilde{\chi}}(H_{\text{eff}}^{(0)}) U^\varepsilon \chi(H^\varepsilon) U^{\varepsilon *} &= \tilde{\tilde{\chi}}(H_{\text{eff}}^\varepsilon) U^\varepsilon \chi(H^\varepsilon) U^{\varepsilon *} + \mathcal{O}(\varepsilon) \\
&= U^\varepsilon \tilde{\tilde{\chi}}(H^\varepsilon) P^\varepsilon \chi(H^\varepsilon) U^{\varepsilon *} + \mathcal{O}(\varepsilon) \\
&= U^\varepsilon P^\varepsilon \tilde{\tilde{\chi}}(H^\varepsilon) \chi(H^\varepsilon) U^{\varepsilon *} + \mathcal{O}(\varepsilon) \\
&= U^\varepsilon \chi(H^\varepsilon) U^{\varepsilon *} + \mathcal{O}(\varepsilon),
\end{aligned}
$$

which shows that

$$
\begin{aligned}
\langle \phi \,|\, H_{\text{eff}}^{(2)} \, \psi^\chi \rangle \;=\; \int_\mathcal{C} \Big(& g_{\text{eff}}^\varepsilon \big((p_{\text{eff}}^\varepsilon \phi)^*, p_{\text{eff}}^\varepsilon \psi^\chi \big) + \phi^* \big(E_{\text{f}} + \varepsilon \, \langle \varphi_{\text{f}} | (\nabla^{\text{v}} W) \varphi_{\text{f}} \rangle_{\mathcal{H}_{\text{f}}} \big) \psi^\chi \\
& + \phi^* \varepsilon^2 \, W^{(2)} \, \psi^\chi - \varepsilon^2 \, \mathcal{M} \big(\Phi^*(\phi), \Phi(\psi^\chi) \big) d\mu_{\text{eff}}^\varepsilon \\
+ \mathcal{O}(\varepsilon^3 & \|\phi\|_{\mathcal{H}_{\text{eff}}} \|\psi\|_{\mathcal{H}_{\text{eff}}}). \quad\quad\quad\quad\quad\quad\quad\quad (55)
\end{aligned}
$$

So now we aim at showing that the same is true for $\langle \phi \,|\, H_{\text{eff}}^\varepsilon \, \psi^\chi \rangle$. In the following, we omit the ε-scripts of $H_{\text{eff}}^\varepsilon, U_1^\varepsilon, U_2^\varepsilon$, and $\tilde{U}_\varepsilon$ and set $\mathcal{H}_{\text{b}} := L^2(\mathcal{C}, d\mu)$. Next we will show that

$$
\begin{aligned}
\langle \phi \,|\, H_{\text{eff}} \, \psi^\chi \rangle_{\mathcal{H}_{\text{eff}}} \;=\; & \langle \tilde{\phi} \,|\, U_0 \, (H_0 + \varepsilon H_1 + \varepsilon^2 H_2) \, U_0^* \, \tilde{\psi}_\chi \rangle_{\mathcal{H}_{\text{b}}} \\
& + \varepsilon \, \langle \tilde{\phi} \,|\, U_0 \big(U_1 \, (H_0 + \varepsilon H_1) + (H_0 + \varepsilon H_1) \, U_1^* \big) U_0^* \, \tilde{\psi}_\chi \rangle_{\mathcal{H}_{\text{b}}} \\
& + \varepsilon^2 \, \langle \tilde{\phi} \,|\, U_0 \, \big(U_1 \, H_0 \, U_1^* + U_2 \, H_0 + H_0 \, U_2^* \big) U_0^* \, \tilde{\psi}_\chi \rangle_{\mathcal{H}_{\text{b}}} \\
& + \mathcal{O}(\varepsilon^3 \|\phi\|_{\mathcal{H}_{\text{eff}}} \|\psi\|_{\mathcal{H}_{\text{eff}}}). \quad\quad\quad\quad (56)
\end{aligned}
$$

By definition of H_{eff} it holds

$$
\begin{aligned}
\langle \phi \,|\, H_{\text{eff}} \, \psi^\chi \rangle_{\mathcal{H}_{\text{eff}}} \;=\; & \langle \tilde{\phi} \,|\, M_{\tilde{\rho}} H_{\text{eff}} M_{\tilde{\rho}}^* \, \tilde{\psi}_\chi \rangle_{\mathcal{H}_{\text{b}}} \;=\; \langle \tilde{\phi} \,|\, U_\varepsilon \, H_\varepsilon \, U_\varepsilon^* \, \tilde{\psi}_\chi \rangle_{\mathcal{H}_{\text{b}}} \\
&= \langle \tilde{\phi} \,|\, U_0 \tilde{U} \, H_\varepsilon \, \tilde{U}^* U_0^* \, \tilde{\psi}_\chi \rangle_{\mathcal{H}_{\text{b}}}.
\end{aligned}
$$

If we could just count the number of ε's after plugging in the expansion of H_ε from Lemma 5 and the one of $\tilde{U}$ from Lemma 6, the claim (56) would be clear. But the expansion of H_ε yields polynomially growing coefficients. So we have to use carefully the estimate (46).

By Lemma 6 it holds $\|u P_0 \tilde{U}\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon))} \lesssim 1$ for each $u \in \{\tilde{U}^*, 1, U_1^*, U_2^*\}$. Since $\tilde{U}^* P_0 = P_\varepsilon \tilde{U}^* P_0$ and $U_2^* P_0 = P_0 U_2^* P_0$ by Lemma 6, $u P_0 \tilde{U}$ satisfies the assumptions on A in Lemma 5 with $m = 0$ for all those u due to the decay properties of P_ε, P_0, and $U_1^* P_0$ from Lemma 2 and Lemma 6. We notice that $\|\chi(H_\varepsilon)\|_{\mathcal{L}(\mathcal{H},\mathcal{D}(H_\varepsilon))} \lesssim 1$ because H_ε is bounded from below and the support of χ is bounded from above, both independently of ε. Hence, using $U_0^* U_\varepsilon = P_0 \tilde{U}$ we may conclude from (46) that

$$\|h\, u\, U_0^* \tilde{\psi}_\chi\|_\mathcal{H} \;=\; \|h\, u\, P_0\, \tilde{U}\, \chi(H_\varepsilon)\, U_\varepsilon^*\, \tilde{\psi}\|_\mathcal{H} \;\lesssim\; \|\psi\|_{\mathcal{H}_{\mathrm{eff}}} \tag{57}$$

for each $h \in \{H_\varepsilon, H_0, H_1, H_2\}$. Furthermore, Lemma 5 implies in the same way that

$$\big\|\big(H_\varepsilon - (H_0 + \varepsilon H_1 + \varepsilon^2 H_2)\big)\tilde{U}^* U_0^* \tilde{\psi}_\chi\big\|_{\mathcal{H}_{\mathrm{eff}}} \;=\; \mathcal{O}(\varepsilon^3).$$

So we have

$$\begin{aligned}
H_\varepsilon\, \tilde{U}^* U_0^*\, \tilde{\psi}_\chi \;&=\; (H_0 + \varepsilon H_1 + \varepsilon^2 H_2)\, \tilde{U}^* U_0^*\, \tilde{\psi}_\chi \;+\; \mathcal{O}(\varepsilon^3 \|\psi\|) \\
&=\; (H_0 + \varepsilon H_1 + \varepsilon^2 H_2)\,(1 + \varepsilon U_1^* + \varepsilon^2 U_2^*) U_0^*\, \tilde{\psi}_\chi \;+\; \mathcal{O}(\varepsilon^3 \|\psi\|) \\
&=\; \Big((H_0 + \varepsilon H_1 + \varepsilon^2 H_2) \\
&\qquad + \varepsilon\,(H_0 + \varepsilon H_1) U_1^* \;+\; \varepsilon^2 H_0 U_2^*\Big) U_0^*\, \tilde{\psi}_\chi \;+\; \mathcal{O}(\varepsilon^3 \|\psi\|).
\end{aligned}$$

For the rest of the proof we write $\mathcal{O}(\varepsilon^l)$ for bounded by $\varepsilon^l \|\phi\|_{\mathcal{H}_{\mathrm{eff}}} \|\psi\|_{\mathcal{H}_{\mathrm{eff}}}$ times a constant independent of ε. The above yields

$$\begin{aligned}
\langle \phi \,|\, H_{\mathrm{eff}}\, \psi \rangle \;&=\; \langle \tilde{\phi} \,|\, U_0 \tilde{U}\, H_\varepsilon\, \tilde{U}^* U_0^*\, \tilde{\psi}_\chi \rangle \\
&=\; \langle \tilde{\phi} \,|\, U_0 \tilde{U}(H_0 + \varepsilon H_1 + \varepsilon^2 H_2)\, U_0^*\, \tilde{\psi}_\chi \rangle \\
&\quad + \varepsilon\, \langle \tilde{\phi} \,|\, U_0 \tilde{U}\,(H_0 + \varepsilon H_1)\, U_1^* U_0^* \tilde{\psi}_\chi \rangle \\
&\quad + \varepsilon^2\, \langle U_0^* \tilde{\phi} \,|\, \tilde{U}\, H_0 U_2\, U_0^* \tilde{\psi}_\chi \rangle \;+\; \mathcal{O}(\varepsilon^3),
\end{aligned}$$

After plugging $\tilde{U} = 1 + \varepsilon U_1 + \varepsilon^2 U_2$ we may drop the terms with three or more ε's in it because of (57). Gathering all the remaining terms we, indeed, end up with (56).

Now we calculate all the terms in (56) separately. By Remark 1

$$\langle \tilde{\phi} \,|\, U_0\, A\, U_0^*\, \tilde{\psi}_\chi \rangle_{\mathcal{H}_{\mathrm{b}}} \;=\; \langle \varphi_{\mathrm{f}} \tilde{\phi} \,|\, A\, \varphi_{\mathrm{f}} \tilde{\psi}_\chi \rangle_\mathcal{H}. \tag{58}$$

for any operator A. Furthermore, the exponential decay of φ_{f} and its derivatives due to the Lemma 6 guarantees that, in the following, all the fiber integrals are bounded in spite of the terms growing polynomially in ν.

We observe that $\tilde{\psi}_\chi = U_0 \tilde{U} \chi(H_\varepsilon) U_\varepsilon^* \tilde{\psi}$ implies that

$$\|H_{\mathrm{eff}}^{(0)} \tilde{\psi}_\chi\|_{\mathcal{H}_{\mathrm{b}}} \lesssim \|H_\varepsilon \chi(H_\varepsilon) U_\varepsilon^* \tilde{\psi}\|_{\mathcal{H}} + \|\chi(H_\varepsilon) U_\varepsilon^* \tilde{\psi}\|_{\mathcal{H}} \lesssim 1$$

because $\|U_0\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon), \mathcal{D}(H_{\mathrm{eff}}^{(0)}))} \lesssim 1$ and $\|\tilde{U}\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon))} \lesssim 1$ by Lemma 6. As explained in Step 1 every differential operator of second order with coefficients in $C_{\mathrm{b}}^\infty(\mathcal{C})$ on $\mathcal{H}_{\mathrm{eff}}$ is operator-bounded by $H_{\mathrm{eff}}^{(0)}$. Therefore derivatives that hit $\tilde{\psi}_\chi$ do not pose any problem, either. These facts will be used throughout the computations below. We write down the calculations via 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. Since $\|\varphi_{\mathrm{f}}\|_{\mathcal{H}_{\mathrm{f}}(q)} = 1$ for all $q \in \mathcal{C}$, Lemma 4 implies

$$2\,\mathrm{Re}\langle \varphi_{\mathrm{f}} | \nabla^{\mathrm{h}} \varphi_{\mathrm{f}} \rangle_{\mathcal{H}_{\mathrm{f}}} = \langle \nabla_\tau^{\mathrm{h}} \varphi_{\mathrm{f}} | \varphi_{\mathrm{f}} \rangle_{\mathcal{H}_{\mathrm{f}}} + \langle \varphi_{\mathrm{f}} | \nabla_\tau^{\mathrm{h}} \varphi_{\mathrm{f}} \rangle_{\mathcal{H}_{\mathrm{f}}} = \left(\mathrm{d}\langle \varphi_{\mathrm{f}} | \varphi_{\mathrm{f}} \rangle_{\mathcal{H}_{\mathrm{f}}}\right)(\tau) = 0.$$

Thus $\langle \varphi_{\mathrm{f}} | \nabla^{\mathrm{h}} \varphi_{\mathrm{f}} \rangle_{\mathcal{H}_{\mathrm{f}}} = \mathrm{Im}\langle \varphi_{\mathrm{f}} | \nabla^{\mathrm{h}} \varphi_{\mathrm{f}} \rangle_{\mathcal{H}_{\mathrm{f}}}$. Therefore the product rule (53) implies

$$\langle \varphi_{\mathrm{f}} \tilde{\phi} \,|\, H_0 \, \varphi_{\mathrm{f}} \tilde{\psi}_\chi \rangle_{\mathcal{H}}$$
$$\overset{(45)}{=} \int_{\mathcal{C}} \tilde{\phi}^* \langle \varphi_{\mathrm{f}} | H_{\mathrm{f}} \varphi_{\mathrm{f}} \rangle_{\mathcal{H}_{\mathrm{f}}} \tilde{\psi}_\chi \, d\mu + \int_{\mathcal{C}} \int_{N_q \mathcal{C}} g(\varepsilon \nabla^{\mathrm{h}} \varphi_{\mathrm{f}}^* \tilde{\phi}^*, \varepsilon \nabla^{\mathrm{h}} \varphi_{\mathrm{f}} \tilde{\psi}_\chi) \, d\nu \, d\mu$$
$$= \int_{\mathcal{C}} \tilde{\phi}^* E_{\mathrm{f}} \tilde{\psi}_\chi \, d\mu + \int_{\mathcal{C}} \int_{N_q \mathcal{C}} |\varphi_{\mathrm{f}}|^2 \, g\big(\varepsilon \mathrm{d}\tilde{\phi}^*, \varepsilon \mathrm{d}\tilde{\psi}_\chi\big) + \varepsilon \, g\big(\varphi_{\mathrm{f}}^* \, \varepsilon \mathrm{d}\tilde{\phi}^*, \tilde{\psi}_\chi \, \nabla^{\mathrm{h}} \varphi_{\mathrm{f}}\big)$$
$$\qquad\qquad + \varepsilon \, g\big(\tilde{\phi}^* \, \nabla^{\mathrm{h}} \varphi_{\mathrm{f}}^*, \varphi_{\mathrm{f}} \, \varepsilon \mathrm{d}\tilde{\psi}_\chi\big) + \varepsilon^2 \, g\big(\tilde{\phi}^* \, \nabla^{\mathrm{h}} \varphi_{\mathrm{f}}^*, \tilde{\psi}_\chi \, \nabla^{\mathrm{h}} \varphi_{\mathrm{f}}\big) \, d\nu \, d\mu$$
$$= \int_{\mathcal{C}} g\big((p_{\mathrm{eff}} \tilde{\phi})^*, p_{\mathrm{eff}} \tilde{\psi}_\chi\big) + \tilde{\phi}^* E_{\mathrm{f}} \tilde{\psi}_\chi + \varepsilon^2 \, \tilde{\phi}^* V_{\mathrm{BH}} \tilde{\psi}_\chi \, d\mu$$
$$\qquad - \varepsilon^2 \int_{\mathcal{C}} g\big((-\mathrm{i}\varepsilon \mathrm{d}\tilde{\phi})^*, \tilde{\psi}_\chi(r_1 + r_2)\big) + g\big(\tilde{\phi}^*(r_1 + r_2)^*, -\mathrm{i}\varepsilon \mathrm{d}\tilde{\psi}_\chi\big) \, d\mu \qquad (59)$$

with

$$V_{\mathrm{BH}} = \int_{N_q \mathcal{C}} g_{\mathrm{eff}}^\varepsilon(\nabla^{\mathrm{h}} \varphi_{\mathrm{f}}^*, (1 - P_0) \nabla^{\mathrm{h}} \varphi_{\mathrm{f}}) \, d\nu,$$

$$p_{\mathrm{eff}}^\varepsilon \psi = -\mathrm{i}\varepsilon \mathrm{d}\psi - \mathrm{Im}\left(\varepsilon \, \langle \varphi_{\mathrm{f}} | \nabla^{\mathrm{h}} \varphi_{\mathrm{f}} \rangle_{\mathcal{H}_{\mathrm{f}}} - \varepsilon^2 \int_{N_q \mathcal{C}} \tfrac{2}{3} \, \varphi_{\mathrm{f}}^* \overline{\mathrm{R}}(\nabla^{\mathrm{v}} \varphi_{\mathrm{f}}, \nu) \nu \, d\nu \right.$$
$$\left. + \varepsilon^2 \, \big\langle \varphi_{\mathrm{f}} \,\big|\, 2\big(\mathcal{W}(\,.\,) - \langle \varphi_{\mathrm{f}} | \mathcal{W}(\,.\,) \varphi_{\mathrm{f}} \rangle_{\mathcal{H}_{\mathrm{f}}}\big) \nabla^{\mathrm{h}} \varphi_{\mathrm{f}} \big\rangle_{\mathcal{H}_{\mathrm{f}}}\right) \psi,$$

as well as $r_1 := \mathrm{Im}\, R_1$ for $R_1 := \big\langle \varphi_{\mathrm{f}} \,\big|\, 2\big(\mathcal{W}(\,.\,) - \langle \varphi_{\mathrm{f}} | \mathcal{W}(\,.\,) \varphi_{\mathrm{f}} \rangle_{\mathcal{H}_{\mathrm{f}}}\big) \nabla^{\mathrm{h}} \varphi_{\mathrm{f}} \big\rangle_{\mathcal{H}_{\mathrm{f}}}$ and $r_2 := \mathrm{Im}\, R_2$ for $R_2 := \int_{N_q \mathcal{C}} \tfrac{2}{3} \, \varphi_{\mathrm{f}}^* \mathrm{R}(\nabla^{\mathrm{v}} \varphi_{\mathrm{f}}, \nu) \nu \, d\nu$. When we split up R_i into real and imaginary part for $i \in \{1, 2\}$, an integration by parts shows

that

$$\int_{\mathcal{C}} g\big((-i\varepsilon d\tilde{\phi})^*, \tilde{\psi}_\chi R_i\big) + g\big(\tilde{\phi}^* R_i^*, -i\varepsilon d\tilde{\psi}_\chi\big) \, d\mu$$

$$= \int_{\mathcal{C}} g\big((-i\varepsilon d\tilde{\phi})^*, \tilde{\psi}_\chi r_i\big) + g\big(\tilde{\phi}^* r_i^*, -i\varepsilon d\tilde{\psi}_\chi\big) \, d\mu \; + \; \mathcal{O}(\varepsilon).$$

Therefore the r_1-terms are cancelled by terms coming from H_1:

$$\langle \varphi_f \tilde{\phi} \,|\, H_1 \, \varphi_f \tilde{\psi}_\chi \rangle_{\mathcal{H}}$$

$$\overset{(45)}{=} \int_{\mathcal{C}} \int_{N_q\mathcal{C}} 2\mathrm{II}(\nu)\big(\varepsilon \nabla^h \varphi_f^* \tilde{\phi}^*, \varepsilon \nabla^h \varphi_f \tilde{\psi}_\chi\big) \; + \; \tilde{\phi}^* \,(\nabla_\nu^v W)|\varphi_f|^2 \, \tilde{\psi}_\chi \, d\nu \, d\mu$$

$$= \int_{\mathcal{C}} \int_{N_q\mathcal{C}} |\varphi_f|^2 \, 2\mathrm{II}(\nu)\big(\varepsilon d\tilde{\phi}^*, \varepsilon d\tilde{\psi}_\chi\big) \; + \; \varepsilon\, 2\mathrm{II}(\nu)\big(\varphi_f^* \, \varepsilon d\tilde{\phi}^*, \tilde{\psi}_\chi \nabla^h \varphi_f\big)$$

$$+ \, \varepsilon\, 2\mathrm{II}(\nu)\big(\tilde{\phi}^* \nabla^h \varphi_f^*, \varphi_f \, \varepsilon d\tilde{\psi}_\chi\big) \; + \; \tilde{\phi}^* \,(\nabla_\nu^v W)|\varphi_f|^2 \, \tilde{\psi}_\chi \, d\nu \, d\mu \; + \; \mathcal{O}(\varepsilon^2)$$

$$= \int_{\mathcal{C}} \langle \varphi_f | 2\mathrm{II}(\,.\,)\big((p_{\mathrm{eff}}\tilde{\phi})^*, p_{\mathrm{eff}}\tilde{\psi}_\chi\big) \varphi_f \rangle_{\mathcal{H}_f} \, d\mu \; + \; \int_{\mathcal{C}} \tilde{\phi}^* \langle \varphi_f | (\nabla_\cdot^v W)\varphi_f \rangle_{\mathcal{H}_f} \, \tilde{\psi}_\chi \, d\mu$$

$$+ \, \varepsilon \int_{\mathcal{C}} g\big((-i\varepsilon d\tilde{\phi})^*, \tilde{\psi}_\chi R_1\big) \; + \; g\big(\tilde{\phi}^* R_1^*, -i\varepsilon d\tilde{\psi}_\chi\big) \, d\mu \; + \; \mathcal{O}(\varepsilon^2), \qquad (60)$$

where we used that $g(\tau_1, \mathcal{W}(\nu)\tau_2) = \mathrm{II}(\nu)(\tau_1, \tau_2) = g(\mathcal{W}(\nu)\tau_1, \tau_2)$ (see the second appendix). At second order we first omit all the terms involving the Riemann tensor:

$$\langle \varphi_f \tilde{\phi} \,|\, H_2 \, \varphi_f \tilde{\psi}_\chi \rangle_{\mathcal{H}} \; - \; \text{'Riemann-terms'}$$

$$\overset{(45)}{=} \int_{\mathcal{C}} \int_{N_q\mathcal{C}} 3g\big(\mathcal{W}(\nu)\varepsilon \nabla^h \varphi_f^* \tilde{\phi}^*, \mathcal{W}(\nu)\varepsilon \nabla^h \varphi_f \tilde{\psi}_\chi\big)$$

$$+ \, \tilde{\phi}^* \,(\tfrac{1}{2}\nabla_{\nu,\nu}^v W + V_{\mathrm{geom}})|\varphi_f|^2 \, \tilde{\psi}_\chi \, d\nu \, d\mu$$

$$= \int_{\mathcal{C}} \langle \varphi_f | 3g\big(\mathcal{W}(\,.\,)\varepsilon d\tilde{\phi}^*, \mathcal{W}(\,.\,)\varepsilon d\tilde{\psi}_\chi\big) \varphi_f \rangle_{\mathcal{H}_f} \, d\mu \; + \; \mathcal{O}(\varepsilon)$$

$$+ \int_{\mathcal{C}} \tilde{\phi}^* \,\big(\langle \varphi_f | (\tfrac{1}{2}\nabla_{\cdot,\cdot}^v W)\varphi_f \rangle_{\mathcal{H}_f} + V_{\mathrm{geom}}\big) \tilde{\psi}_\chi \, d\mu$$

$$= \int_{\mathcal{C}} \langle \varphi_f | 3g\big(\mathcal{W}(\,.\,)(p_{\mathrm{eff}}\tilde{\psi}_\chi)^*, \mathcal{W}(\,.\,)p_{\mathrm{eff}}\tilde{\psi}_\chi\big) \varphi_f \rangle_{\mathcal{H}_f} \, d\mu$$

$$+ \int_{\mathcal{C}} \tilde{\phi}^* \,\big(\langle \varphi_f | (\tfrac{1}{2}\nabla_{\cdot,\cdot}^v W)\varphi_f \rangle_{\mathcal{H}_f} + V_{\mathrm{geom}}\big) \tilde{\psi}_\chi \, d\mu \; + \; \mathcal{O}(\varepsilon), \qquad (61)$$

where we used that $-i\varepsilon d\tilde{\psi}_\chi = p_{\mathrm{eff}}\tilde{\psi}_\chi + \mathcal{O}(\varepsilon)$ in the last step. Now we take care of the omitted second order terms. Noticing that $\nabla^v \tilde{\psi}_\chi \varphi_f = \tilde{\psi}_\chi \nabla^v \varphi_f$

we have

'Riemann-terms'

$$\overset{(45)}{=} \int_{\mathcal{C}} \int_{N_q\mathcal{C}} \overline{\mathcal{R}}\big(\varepsilon\nabla^{\mathrm{h}}\varphi_{\mathrm{f}}^*\tilde{\phi}^*, \nu, \varepsilon\nabla^{\mathrm{h}}\varphi_{\mathrm{f}}\tilde{\psi}_\chi, \nu\big) \;+\; \tfrac{2}{3}\,\overline{\mathcal{R}}\big(\varepsilon\nabla^{\mathrm{h}}\varphi_{\mathrm{f}}^*\tilde{\phi}^*, \nu, \nabla^{\mathrm{v}}\varphi_{\mathrm{f}}\tilde{\psi}_\chi, \nu\big)$$

$$+ \tfrac{2}{3}\,\overline{\mathcal{R}}\big(\nabla^{\mathrm{v}}\varphi_{\mathrm{f}}^*\tilde{\phi}^*, \nu, \varepsilon\nabla^{\mathrm{h}}\varphi_{\mathrm{f}}\tilde{\psi}_\chi, \nu\big) \;+\; \tfrac{1}{3}\,\overline{\mathcal{R}}\big(\nabla^{\mathrm{v}}\varphi_{\mathrm{f}}^*\tilde{\phi}^*, \nu, \nabla^{\mathrm{v}}\varphi_{\mathrm{f}}\tilde{\psi}_\chi, \nu\big)\, d\nu\, d\mu$$

$$= \int_{\mathcal{C}} \int_{N_q\mathcal{C}} |\varphi_{\mathrm{f}}|^2\, \overline{\mathcal{R}}\big(\varepsilon\mathrm{d}\tilde{\phi}^*, \nu, \varepsilon\mathrm{d}\tilde{\psi}_\chi, \nu\big) \;+\; \tfrac{2}{3}\,\overline{\mathcal{R}}\big(\varphi_{\mathrm{f}}^*\varepsilon\mathrm{d}\tilde{\phi}^*, \nu, \tilde{\psi}_\chi\nabla^{\mathrm{v}}\varphi_{\mathrm{f}}, \nu\big)$$

$$+\tfrac{2}{3}\,\overline{\mathcal{R}}\big(\tilde{\phi}^*\nabla^{\mathrm{v}}\varphi_{\mathrm{f}}^*, \nu, \varphi_{\mathrm{f}}\,\varepsilon\mathrm{d}\tilde{\psi}_\chi, \nu\big) \;+\; \tfrac{1}{3}\,\tilde{\phi}^*\overline{\mathcal{R}}\big(\nabla^{\mathrm{v}}\varphi_{\mathrm{f}}^*, \nu, \nabla^{\mathrm{v}}\varphi_{\mathrm{f}}, \nu\big)\tilde{\psi}_\chi\, d\nu\, d\mu \;+\; \mathcal{O}(\varepsilon)$$

$$= \int_{\mathcal{C}} \big\langle \varphi_{\mathrm{f}} \,\big|\, \overline{\mathcal{R}}\big(\varepsilon\mathrm{d}\tilde{\phi}^*, .\,, \varepsilon\mathrm{d}\tilde{\psi}_\chi, .\big)\varphi_{\mathrm{f}} \big\rangle_{\mathcal{H}_{\mathrm{f}}}\, d\mu \;+\; \int_{\mathcal{C}} \tilde{\phi}^* V_{\mathrm{amb}}\, \tilde{\psi}_\chi\, d\mu$$

$$+ \int_{\mathcal{C}} g\big((-\mathrm{i}\varepsilon\mathrm{d}\tilde{\phi})^*, \tilde{\psi}_\chi R_2\big) \;+\; g\big(\tilde{\phi}^* R_2^*, -\mathrm{i}\varepsilon\mathrm{d}\tilde{\psi}_\chi\big)\, d\mu \;+\; \mathcal{O}(\varepsilon) \qquad (62)$$

with $V_{\mathrm{amb}} = \int_{N_q\mathcal{C}} \tfrac{1}{3}\,\overline{\mathcal{R}}\big(\nabla^{\mathrm{v}}\varphi_{\mathrm{f}}^*, \nu, \nabla^{\mathrm{v}}\varphi_{\mathrm{f}}, \nu\big)\, d\nu$. Again replacing $-\mathrm{i}\varepsilon\mathrm{d}\tilde{\psi}_\chi$ with $p_{\mathrm{eff}}\tilde{\psi}_\chi$ and g with g_{eff} yields errors of order ε only. In view of (58)-(62), we have

$$\langle \tilde{\phi} \,|\, U_0\, (H_0 \,+\, \varepsilon H_1 \,+\, \varepsilon^2 H_2)\, U_0^*\, \tilde{\psi}_\chi\rangle_{\mathcal{H}_{\mathrm{b}}}$$

$$= \int_{\mathcal{C}} g_{\mathrm{eff}}^\varepsilon\big((p_{\mathrm{eff}}\tilde{\phi})^*, p_{\mathrm{eff}}\tilde{\psi}_\chi\big) \;+\; \tilde{\phi}^*\, E_{\mathrm{f}}\, \tilde{\psi}_\chi$$

$$+\, \tilde{\phi}^*\, \big(\varepsilon\langle\varphi_{\mathrm{f}}|\nabla^{\mathrm{v}}_. W\varphi_{\mathrm{f}}\rangle_{\mathcal{H}_{\mathrm{f}}} + \varepsilon^2 W^{(2)}\big)\, \tilde{\psi}_\chi\, d\mu \;+\; \mathcal{O}(\varepsilon^3) \qquad (63)$$

with

$$g_{\mathrm{eff}}^\varepsilon(\tau_1, \tau_2) \;=\; g(\tau_1, \tau_2) \;+\; \varepsilon\, \big\langle\, \varphi_{\mathrm{f}} \,\big|\, 2\mathrm{II}(\,.\,)(\tau_1, \tau_2)\, \varphi_{\mathrm{f}}\, \big\rangle_{\mathcal{H}_{\mathrm{f}}}$$

$$+\, \varepsilon^2\, \Big\langle\, \varphi_{\mathrm{f}} \,\Big|\, 3g\big(\mathcal{W}(\,.\,)\tau_1, \mathcal{W}(\,.\,)\tau_2\big)\, \varphi_{\mathrm{f}} \;+\; \overline{\mathcal{R}}\big(\tau_1, .\,, \tau_2, .\big)\varphi_{\mathrm{f}}\, \Big\rangle_{\mathcal{H}_{\mathrm{f}}}.$$

We define $P_0^\perp := (1 - P_0)$. Before we deal with the corrections by U_1 and U_2 in (56), we notice that due to $P_0 = U_0^* U_0^*$ and $P_0^\perp U_0^* = 0$

$$P_0^\perp\big([-\varepsilon\Delta_{\mathrm{h}}, P_0] \,+\, H_1\big)\, U_0^*\tilde{\psi}_\chi$$

$$\overset{(45)}{=} \;\; P_0^\perp\Big([-\varepsilon\Delta_{\mathrm{h}}, U_0^* U_0] \,-\, \mathrm{tr}_{\mathcal{C}}\, \varepsilon\nabla^{\mathrm{h}}\mathcal{W}(\nu)\, \varepsilon\nabla^{\mathrm{h}} \,+\, (\nabla^{\mathrm{v}}_\nu W)\Big)\, U_0^*\tilde{\psi}_\chi$$

$$= \;\; P_0^\perp\Big((\nabla^{\mathrm{v}}_\nu W) \,-\, \mathrm{tr}_{\mathcal{C}}\big(2(\nabla^{\mathrm{h}}\varphi_{\mathrm{f}})U_0 + \varepsilon\nabla^{\mathrm{h}}\mathcal{W}(\nu)\big)\, \varepsilon\nabla^{\mathrm{h}}\Big)\, U_0^*\tilde{\psi}_\chi \;+\; \mathcal{O}(\varepsilon)$$

$$= \;\; P_0^\perp\Big(\varphi_{\mathrm{f}}(\nabla^{\mathrm{v}}_\nu W)\tilde{\psi}_\chi \,-\, 2g(\nabla^{\mathrm{h}}\varphi_{\mathrm{f}}^*, \varepsilon\mathrm{d}\tilde{\psi}_\chi) \,-\, \varphi_{\mathrm{f}}\, \mathrm{tr}_{\mathcal{C}}\, \mathcal{W}(\nu)\varepsilon^2\nabla\mathrm{d}\tilde{\psi}_\chi\Big) \;+\; \mathcal{O}(\varepsilon)$$

$$= \;\; P_0^\perp\, \Psi(\varepsilon\nabla\mathrm{d}\tilde{\psi}_\chi, \mathrm{d}\tilde{\psi}_\chi, \tilde{\psi}_\chi) \;+\; \mathcal{O}(\varepsilon). \qquad (64)$$

with $\Psi(A, p, \phi) = -\,\varphi_{\mathrm{f}}\, \mathrm{tr}_{\mathcal{C}}\big(\mathcal{W}(\nu)A\big) \,-\, 2g_{\mathrm{eff}}^\varepsilon\big(\nabla^{\mathrm{h}}\varphi_{\mathrm{f}}^*, p\big) \,+\, \varphi_{\mathrm{f}}(\nabla^{\mathrm{v}}_\nu W)\phi.$

We note that $U_0^* \tilde{\psi}_\chi = B^\varepsilon U^* \tilde{\psi}$ with $B^\varepsilon = P_0 \tilde{U} \chi(H_\varepsilon)$. So we may apply (47) und (48) in the following. Since $U_0 = U_0 P_0$ by definition and we know from Lemma 6 that $P_0 U_1 P_0 = 0$, the first corrections by U_1 are an order of ε higher than expected:

$$\left\langle \tilde{\phi} \,\middle|\, U_0 \left((H_0 + \varepsilon H_1) U_1^* + U_1 (H_0 + \varepsilon H_1) \right) U_0^* \tilde{\psi}_\chi \right\rangle_{\mathcal{H}_\mathrm{b}}$$

$$= \left\langle \tilde{\phi} \,\middle|\, U_0 \left(([P_0, H_0] + \varepsilon H_1) U_1^* + U_1 ([H_0, P_0] + \varepsilon H_1) \right) U_0^* \tilde{\psi}_\chi \right\rangle_{\mathcal{H}_\mathrm{b}}$$

$$= \varepsilon \left\langle \tilde{\phi} \,\middle|\, U_0 \left(([\varepsilon \Delta_\mathrm{h}, P_0] + H_1) U_1^* + U_1 ([-\varepsilon \Delta_\mathrm{h}, P_0] + H_1) P_0 \right) U_0^* \tilde{\psi}_\chi \right\rangle_{\mathcal{H}_\mathrm{b}}$$

$$\overset{(48)}{=} -\varepsilon \left\langle \tilde{\phi} \,\middle|\, U_0 \left([\varepsilon \Delta_\mathrm{h}, P_0] + H_1 \right) R_{H_\mathrm{f}}(E_\mathrm{f}) \left([-\varepsilon \Delta_\mathrm{h}, P_0] + H_1 \right) U_0^* \tilde{\psi}_\chi \right\rangle_{\mathcal{H}_\mathrm{b}}$$

$$\qquad - \varepsilon \langle \tilde{\phi} \,|\, U_0 U_1 (H_\mathrm{f} - E_\mathrm{f}) U_1^* U_0^* \tilde{\psi}_\chi \rangle_{\mathcal{H}_\mathrm{b}}$$

$$\overset{(64)}{=} -\varepsilon \left\langle \Psi(\varepsilon^2 \nabla \mathrm{d} \tilde{\phi}, \varepsilon \mathrm{d} \tilde{\phi}, \tilde{\phi}) \,\middle|\, R_{H_\mathrm{f}}(E_\mathrm{f}) \, \Psi(\varepsilon^2 \nabla \mathrm{d} \tilde{\psi}_\chi, \varepsilon \mathrm{d} \tilde{\psi}_\chi, \tilde{\psi}_\chi) \right\rangle_{\mathcal{H}_\mathrm{b}}$$

$$\qquad - \varepsilon \langle \tilde{\phi} \,|\, U_0 U_1 (H_\mathrm{f} - E_\mathrm{f}) U_1^* U_0^* \tilde{\psi}_\chi \rangle_{\mathcal{H}_\mathrm{b}}$$

$$= -\varepsilon \int_\mathcal{C} \mathcal{M}\big(\Psi^*(\varepsilon^2 \nabla \mathrm{d} \tilde{\phi}, \varepsilon \mathrm{d} \tilde{\phi}, \tilde{\phi}), \Psi(\varepsilon^2 \nabla \mathrm{d} \tilde{\psi}_\chi, \varepsilon \mathrm{d} \tilde{\psi}_\chi, \tilde{\psi}_\chi)) \big) \, d\mu$$

$$\qquad - \varepsilon \langle \tilde{\phi} \,|\, U_0 U_1 (H_\mathrm{f} - E_\mathrm{f}) U_1^* U_0^* \tilde{\psi}_\chi \rangle_{\mathcal{H}_\mathrm{b}}. \tag{65}$$

with $\mathcal{M}(\Phi^*, \Psi) = \left\langle \Phi \,\middle|\, (1 - P_0) (H_\mathrm{f} - E_\mathrm{f})^{-1} (1 - P_0) \Psi \right\rangle_{\mathcal{H}_\mathrm{f}}$. Furthermore,

$$\langle \tilde{\phi} \,|\, U_0 \left(U_2 H_0 + H_0 U_2^* \right) U_0^* \tilde{\psi}_\chi \rangle_{\mathcal{H}_\mathrm{b}}$$

$$= \langle U_0^* \tilde{\phi} \,|\, P_0 \big(U_2 (-\varepsilon^2 \Delta_\mathrm{h} + H_\mathrm{f}) + (-\varepsilon^2 \Delta_\mathrm{h} + H_\mathrm{f}) U_2^* \big) P_0 U_0^* \tilde{\psi}_\chi \rangle_{\mathcal{H}_\mathrm{b}}$$

$$= \langle U_0^* \tilde{\phi} \,|\, \big(P_0 U_2 (-\varepsilon^2 \Delta_\mathrm{h} + E_\mathrm{f}) P_0 + P_0 (-\varepsilon^2 \Delta_\mathrm{h} + E_\mathrm{f}) U_2^* P_0 \big) U_0^* \tilde{\psi}_\chi \rangle_{\mathcal{H}_\mathrm{b}}$$

$$\overset{(47)}{=} \langle U_0^* \tilde{\phi} \,|\, P_0 (U_2 + U_2^*) P_0 (-\varepsilon^2 \Delta_\mathrm{h} + E_\mathrm{f}) U_0^* \tilde{\psi}_\chi \rangle_{\mathcal{H}_\mathrm{b}} + \mathcal{O}(\varepsilon)$$

$$= - \langle U_0^* \tilde{\phi} \,|\, P_0 U_1 U_1^* P_0 (-\varepsilon^2 \Delta_\mathrm{h} + E_\mathrm{f}) U_0^* \tilde{\psi}_\chi \rangle_{\mathcal{H}_\mathrm{b}} + \mathcal{O}(\varepsilon), \tag{66}$$

because $\tilde{U} = 1 + \varepsilon U_1 + \varepsilon^2 U_2$ 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 (66) and the second term from (65):

$$\left\langle \tilde{\phi} \,\middle|\, U_0 U_1 H_0 U_1^* U_0^* \tilde{\psi}_\chi \right\rangle_{\mathcal{H}_\mathrm{b}}$$

$$= \langle \tilde{\phi} \,|\, U_0 U_1 (-\varepsilon^2 \Delta_\mathrm{h} + H_\mathrm{f}) U_1^* U_0^* \tilde{\psi}_\chi \rangle_{\mathcal{H}_\mathrm{b}}$$

$$= \langle \tilde{\phi} \,|\, U_0 U_1 (H_\mathrm{f} - E_\mathrm{f}) U_1^* U_0^* \tilde{\psi}_\chi + U_0 U_1 (-\varepsilon^2 \Delta_\mathrm{h} + E_\mathrm{f}) U_1^* P_0 U_0^* \tilde{\psi}_\chi \rangle_{\mathcal{H}_\mathrm{b}}$$

$$\overset{(47)}{=} \langle \tilde{\phi} \,|\, U_0 U_1 (H_\mathrm{f} - E_\mathrm{f}) U_1^* U_0^* \tilde{\psi}_\chi \rangle_{\mathcal{H}_\mathrm{b}}$$

$$\qquad + \langle \tilde{\phi} \,|\, U_0 U_1 U_1^* P_0 (-\varepsilon^2 \Delta_\mathrm{h} + E_\mathrm{f}) U_0^* \tilde{\psi}_\chi \rangle_{\mathcal{H}_\mathrm{b}} + \mathcal{O}(\varepsilon). \tag{67}$$

We gather the terms from (63) to (67) and replace $\mathrm{d}\tilde{\psi}_\chi$ by $p_{\mathrm{eff}}^\varepsilon \tilde{\psi}_\chi$ in the argument of Ψ, which only yields an error of order ε^3. Then we obtain that $\langle\, \tilde{\phi} \,|\, H_{\mathrm{eff}}^\varepsilon\, \tilde{\psi}_\chi \,\rangle$ equals the right-hand side of (55) up to errors of order ε, only with $d\mu$ instead of $d\mu_{\mathrm{eff}}$. Here $\tilde{\psi} = M_{\tilde{\rho}}\psi$ enters. By Lemma 1 $M_{\tilde{\rho}}$ interchanges the former with the latter but may add extra terms. However, g and g_{eff} coincide at leading order and so do their associated volume measures. Therefore $\mathrm{d}(\ln\tilde{\rho})$ and $\Delta_{\mathcal{C}}\ln\tilde{\rho}$ are of order ε. This shows that the extra potential from Lemma 1, given by $-\frac{\varepsilon^2}{4}\,g\big(\mathrm{d}(\ln\tilde{\rho}),\mathrm{d}(\ln\tilde{\rho})\big) + \frac{\varepsilon^2}{2}\Delta_{\mathcal{C}}(\ln\tilde{\rho})$, is of order ε^3. Exploiting $\mathrm{d}(\ln\tilde{\rho}) = \mathcal{O}(\varepsilon)$ we easily obtain that all the other extra terms are also only of order ε^3, which finishes the proof of Step 3.

Step 4: It holds $\|(H_{\mathrm{eff}}^\varepsilon - H_{\mathrm{eff}}^{(2)})\chi(H_{\mathrm{eff}}^\varepsilon)\|_{\mathcal{L}(\mathcal{H}_{\mathrm{eff}})} = \mathcal{O}(\varepsilon^3)$.

The spectral calculus implies $\chi(H_{\mathrm{eff}}^\varepsilon) = \tilde{\chi}^2(H_{\mathrm{eff}}^\varepsilon)\chi(H_{\mathrm{eff}}^\varepsilon)$. Furthermore, in view of Corollary 5, U^ε satisfies the assumptions on B in Lemma 7 c) i) with $\delta = \varepsilon^3$ and c) ii) with $\delta = \varepsilon$. Thus in the norm of $\mathcal{L}\big(\mathcal{H}_{\mathrm{eff}},\mathcal{D}(H_{\mathrm{eff}}^\varepsilon)\big)$ it holds

$$
\begin{aligned}
\tilde{\chi}^2(H_{\mathrm{eff}}^\varepsilon) &= U^\varepsilon\tilde{\chi}(H^\varepsilon)U^{\varepsilon*}\,\tilde{\chi}(H_{\mathrm{eff}}^\varepsilon) + \big(\tilde{\chi}(H_{\mathrm{eff}}^\varepsilon) - U^\varepsilon\tilde{\chi}(H^\varepsilon)U^{\varepsilon*}\big)^2 \\
&\quad + \big(\tilde{\chi}(H_{\mathrm{eff}}^\varepsilon) - U^\varepsilon\tilde{\chi}(H^\varepsilon)U^{\varepsilon*}\big)\,U^\varepsilon\tilde{\chi}(H^\varepsilon)U^{\varepsilon*} \\
&= U^\varepsilon\tilde{\chi}(H^\varepsilon)U^{\varepsilon*}\,\tilde{\chi}(H_{\mathrm{eff}}^\varepsilon) + \mathcal{O}(\varepsilon^4) \\
&\quad + \big(\tilde{\chi}(H_{\mathrm{eff}}^\varepsilon) - U^\varepsilon\tilde{\chi}(H^\varepsilon)U^{\varepsilon*}\big)\,U^\varepsilon\tilde{\tilde{\chi}}^2(H^\varepsilon)\tilde{\chi}(H^\varepsilon)U^{\varepsilon*} \\
&= U^\varepsilon\tilde{\chi}(H^\varepsilon)U^{\varepsilon*}\,\tilde{\chi}(H_{\mathrm{eff}}^\varepsilon) + \mathcal{O}(\varepsilon^3). \qquad (68)
\end{aligned}
$$

So we have

$$
\|\,\chi(H_{\mathrm{eff}}^\varepsilon) - U^\varepsilon\tilde{\chi}(H^\varepsilon)U^{\varepsilon*}\,\chi(H_{\mathrm{eff}}^\varepsilon)\|_{\mathcal{L}(\mathcal{H}_{\mathrm{eff}},\mathcal{D}(H_{\mathrm{eff}}^\varepsilon))} = \mathcal{O}(\varepsilon^3).
$$

Now Step 4 follows from Step 3 and $\mathcal{D}(H_{\mathrm{eff}}^{(2)}) = \mathcal{D}(H_{\mathrm{eff}}^\varepsilon)$ due to Step 2.

Step 5: It holds $\|(H_{\mathrm{eff}}^\varepsilon - H_{\mathrm{eff}}^{(2)})\chi(H_{\mathrm{eff}}^{(2)})\|_{\mathcal{L}(\mathcal{H}_{\mathrm{eff}})} = \mathcal{O}(\varepsilon^3)$.

We note that Step 1 & 2 imply that $\|H_{\mathrm{eff}}^\varepsilon - H_{\mathrm{eff}}^{(2)}\|_{\mathcal{L}(\mathcal{D}(H_{\mathrm{eff}}^\varepsilon),\mathcal{H}_{\mathrm{eff}})} = \mathcal{O}(\varepsilon)$. So in the norm of $\mathcal{L}\big(\mathcal{H}_{\mathrm{eff}},\mathcal{D}(H_{\mathrm{eff}}^\varepsilon)\big)$ it holds that

$$
\begin{aligned}
\tilde{\chi}^3(H_{\mathrm{eff}}^{(2)}) &= \tilde{\chi}(H_{\mathrm{eff}}^\varepsilon)\,\tilde{\chi}^2(H_{\mathrm{eff}}^{(2)}) + \big(\tilde{\chi}(H_{\mathrm{eff}}^{(2)}) - \tilde{\chi}(H_{\mathrm{eff}}^\varepsilon)\big)^3 \\
&\quad + \big(\tilde{\chi}(H_{\mathrm{eff}}^{(2)}) - \tilde{\chi}(H_{\mathrm{eff}}^\varepsilon)\big)^2\,\tilde{\chi}(H_{\mathrm{eff}}^\varepsilon) \\
&\quad + \big(\tilde{\chi}(H_{\mathrm{eff}}^{(2)}) - \tilde{\chi}(H_{\mathrm{eff}}^\varepsilon)\big)\,\tilde{\chi}(H_{\mathrm{eff}}^\varepsilon)\,\tilde{\chi}(H_{\mathrm{eff}}^{(2)}) \\
&= \tilde{\chi}(H_{\mathrm{eff}}^\varepsilon)\,\tilde{\chi}^2(H_{\mathrm{eff}}^{(2)}) + \mathcal{O}(\varepsilon^3)
\end{aligned}
$$

by Lemma 7 b) and Step 2 & 4. Hence, Step 5 can be reduced to Step 4 in the same way as we reduced Step 4 to Step 3.

Theorem 2 is entailed by Step 3 to 5 and the remark preceding Step 1. $\qquad\square$

PROOF OF LEMMA 7:

We want to apply the so called Helffer-Sjöstrand formula (see [9], chapter 2) to χ_1. It states that for any $\chi \in C_0^\infty(\mathbb{R})$

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

where $R_H(z) := (H - z)^{-1}$ denotes the resolvent and $\tilde{\chi} : \mathbb{C} \to \mathbb{C}$ is a so-called almost analytic extension of χ. We emphasize that by dz we mean the usual volume measure 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 $\operatorname{supp} \tau \subset [-2, 2]$ and $l \geq 2$. Then obviously $\tilde{\chi} = \chi$ for $y = 0$ and there is $C_\chi < \infty$ depending only on χ such that

$$\partial_{\bar{z}} \tilde{\chi}(z) \; := \; \partial_x \tilde{\chi} + i \partial_y \tilde{\chi} \; \leq \; C_\chi \, |\operatorname{Im} z|^l, \tag{69}$$

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

$$\left\| R_H(z) \right\|_{\mathcal{L}(\mathcal{D}(H^j), \mathcal{D}(H^{j+1}))} \; \leq \; \frac{\sqrt{1 + 2|\operatorname{Im} z|^2 + 2|z|^2}}{|\operatorname{Im} z|} \tag{70}$$

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

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

Now by the Helffer-Sjöstrand formula

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

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

$$\big\|[\chi_1(H), A]\, \chi_2(H)\big\|_{\mathcal{L}(\mathcal{D}(H^{l-1}), \mathcal{D}(H^{m+1}))}$$

$$\leq \quad \frac{1}{\pi} \int_{\mathbb{C}} |\partial_{\bar{z}}\tilde{\chi}_1(z)|\, \|R_H(z)\|_{\mathcal{L}(\mathcal{D}(H^m), \mathcal{D}(H^{m+1}))}$$

$$\times \big\|[H, A]\, \chi_2(H)\big\|_{\mathcal{L}(\mathcal{D}(H^l), \mathcal{D}(H^m))} \|R_H(z)\|_{\mathcal{L}(\mathcal{D}(H^{l-1}), \mathcal{D}(H^l))}\, dz$$

$$\overset{(69),(70)}{\leq} \quad C_{\chi_1} \delta \int_{\mathrm{supp}\tilde{\chi}_1} |\mathrm{Im}z|^2 \frac{1 + 2|\mathrm{Im}z|^2 + 2|z|^2}{|\mathrm{Im}z|^2}\, dz$$

$$\leq \quad C\,\delta,$$

with a C depending only on C_{χ_1} and the support of $\tilde{\chi}_1$. This shows a). The proof of b) can be carried out analogously because

$$\big(\chi_1(H) - \chi_1(\tilde{H})\big)\chi_2(\tilde{H}) \;=\; \frac{1}{\pi} \int_{\mathbb{C}} \partial_{\bar{z}}\tilde{\chi}_1(z)\, \big(R_H(z) - R_{\tilde{H}}(z)\big)\, dz\, \chi_2(\tilde{H})$$

$$=\; \frac{1}{\pi} \int_{\mathbb{C}} \partial_{\bar{z}}\tilde{\chi}_1(z)\, R_H(z)(\tilde{H} - H)\, R_{\tilde{H}}(z)\, dz\, \chi_2(\tilde{H})$$

$$=\; \frac{1}{\pi} \int_{\mathbb{C}} \partial_{\bar{z}}\tilde{\chi}_1(z)\, R_H(z)(\tilde{H} - H)\, \chi_2(\tilde{H})\, R_{\tilde{H}}(z)\, dz.$$

due to the Helffer-Sjöstrand formula. For c) the formula yields:

$$\chi_1(\tilde{H}) - B\chi_1(H)B^* \;=\; \frac{1}{\pi} \int_{\mathbb{C}} \partial_{\bar{z}}\tilde{\chi}_1(z)\big(R_{\tilde{H}}(z) - BR_H(z)B^*\big)\, dz. \qquad (71)$$

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

$$R_{\tilde{H}}(z) - BR_H(z)B^* \;=\; R_{\tilde{H}}(z)\big(1 - (BHB^* - z)BR_H(z)B^*\big)$$

$$=\; R_{\tilde{H}}(z)\big(1 - B(H - z)AR_H(z)B^*\big)$$

$$=\; R_{\tilde{H}}(z)\big(1 - BAB^* - B[H, A]R_H(z)B^*\big)$$

$$=\; -R_{\tilde{H}}(z)\, B[H, A]R_H(z)B^*. \qquad (72)$$

For the second part of c) we observe that $A^2 = A$ entails $A[H, A]A = 0$. Then we may derive from (72) that

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

$$=\; -R_{\tilde{H}}(z)\, BA[H, A](1 - A)[R_H(z), A]B^*$$

$$=\; R_{\tilde{H}}(z)\, BA[H, A]R_H(z)[H, A]R_H(z)B^*$$

$$=\; R_{\tilde{H}}(z)\, B[H, A]R_H(z)[H, A]R_H(z)B^*.$$

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We will write C_B for a constant depending only on $\|B\|_{\mathcal{L}(\mathcal{D}(H^l),\mathcal{D}(\tilde{H}^l))}$ and $\|B^*\|_{\mathcal{L}(\mathcal{D}(\tilde{H}^l),\mathcal{D}(H^l))}$ for $l \leq m$. We note that the estimate (70) holds true with H replaced by $\tilde{H}$ because $\tilde{H}$ is assumed to be self-adjoint. Hence, with $B \in \mathcal{L}\big(\mathcal{D}(H^{m-1}),\mathcal{D}(\tilde{H}^{m-1})\big)$ and $B^* \in \mathcal{L}\big(\mathcal{D}(\tilde{H}^{m-1}),\mathcal{D}(H^{m-1})\big)$ we obtain

$$
\begin{aligned}
&\big\|R_{\tilde{H}}(z) - BR_H(z)B^*\big\|_{\mathcal{L}(\mathcal{D}(\tilde{H}^{m-1}),\mathcal{D}(\tilde{H}^m))} \\
&= \ \big\|R_{\tilde{H}}(z)B\,[H,A]R_H(z)\,[H,A]R_H(z)\,B^*\big\|_{\mathcal{L}(\mathcal{D}(\tilde{H}^{m-1}),\mathcal{D}(\tilde{H}^m))} \\
&\leq \ C_B \frac{(1+2|\mathrm{Im}z|^2+2|z|^2)^{3/2}}{|\mathrm{Im}z|^3}\,\|[H,A]\|^2_{\mathcal{L}(\mathcal{D}(H^m),\mathcal{D}(H^{m-1}))} \\
&\leq \ C_B\,\delta^2\,\frac{(1+2|\mathrm{Im}z|^2+2|z|^2)^{3/2}}{|\mathrm{Im}z|^3}
\end{aligned}
$$

by assumption. Together with (71) this yields the claim as in a) when we put $l=3$ in the choice of the almost analytic extension.

For the first part of c) we compute

$$
\begin{aligned}
B^*\big(R_{\tilde{H}}(z)-BR_H(z)B^*\big)B\,\chi_2^2(H) \\
= \ -B^*R_{\tilde{H}}(z)\,B[H,A]R_H(z)A\chi_2(H)\chi_2(H) \\
= \ -B^*R_{\tilde{H}}(z)\,B[H,A]R_H(z)\big(\chi_2(H)A+[A,\chi_2(H)]\big)\chi_2(H). \quad (73)
\end{aligned}
$$

Then, on the one hand, $B \in \mathcal{L}\big(\mathcal{D}(H^{m-1}),\mathcal{D}(\tilde{H}^{m-1})\big)$ implies

$$
\begin{aligned}
&\|R_{\tilde{H}}(z)B\,[H,A]R_H(z)\,\chi_2(H)A\chi_2(H)\|_{\mathcal{L}(\mathcal{H},\mathcal{D}(\tilde{H}^m))} \\
&= \ \|R_{\tilde{H}}(z)B\,[H,A]\chi_2(H)\,R_H(z)A\chi_2(H)\|_{\mathcal{L}(\mathcal{H},\mathcal{D}(\tilde{H}^m))} \\
&\leq \ C_B \frac{\sqrt{1+2|\mathrm{Im}z|^2+2|z|^2}}{|\mathrm{Im}z|}\,\|[H,A]\chi_2(H)\|_{\mathcal{L}(\mathcal{H},\mathcal{D}(H^{m-1}))}\,|\mathrm{Im}z|^{-1} \\
&\leq \ C_B\,\delta\,\frac{\sqrt{1+2|\mathrm{Im}z|^2+2|z|^2}}{|\mathrm{Im}z|^2}
\end{aligned}
$$

by the assumption on the commutator term. On the other hand, the assumptions on B and B^* imply that

$$
\begin{aligned}
&\|R_{\tilde{H}}(z)\,B[H,A]R_H(z)\,[A,\chi_2(H)]\chi_2(H)\|_{\mathcal{L}(\mathcal{H},\mathcal{D}(\tilde{H}^m))} \\
&= \ \|R_{\tilde{H}}(z)\,B(HB^*B-B^*BH)R_H(z)\,[A,\chi_2(H)]\chi_2(H)\|_{\mathcal{L}(\mathcal{H},\mathcal{D}(\tilde{H}^m))} \\
&\leq \ C_B \frac{2(1+2|\mathrm{Im}z|^2+2|z|^2)}{|\mathrm{Im}z|^2}\,\|[A,\chi_2(H)]\chi_2(H)\|_{\mathcal{L}(\mathcal{H},\mathcal{D}(H^{m-1}))} \\
&\leq \ C_{B,\chi_2}\,\delta\,\frac{2(1+2|\mathrm{Im}z|^2+2|z|^2)}{|\mathrm{Im}z|^2},
\end{aligned}
$$

where C_{B,χ_2} depends also on χ_2 because in the last step we used that H, A, and χ_2 satisfy the assumptions of a). After plugging (73) into (71) the latter two estimates allow us to deduce the first part of c) analogously with a). $\square$

3.4 Proof of the approximation of eigenvalues

With Theorem 2, Corollary 5, and Lemma 7 we have already everything at hand we need to prove Theorem 3, which relates the spectra of H^ε and $H_{\text{eff}}^{(2)}$.

PROOF OF THEOREM 3 (SECTION 2.3):

We fix $E < \infty$ and set $E_- := \min\{\inf \sigma(H^\varepsilon), \inf \sigma(H_{\text{eff}}^{(2)})\} - 1$. Let χ be the characteristic function of $[E_-, E]$ and $\tilde\chi \in C_0^\infty(\mathbb{R})$ with $\tilde\chi|_{[E_-,E]} \equiv 1$.

To show a) i) we assume we are given a family of eigenvalues (E_ε) of $H_{\text{eff}}^{(2)}$ with $\limsup E_\varepsilon < E$ and a corresponding family of eigenfunctions (ψ_ε). Since ψ_ε is an eigenfunction of $H_{\text{eff}}^{(2)}$, we have that $\psi_\varepsilon = \chi(H_{\text{eff}}^{(2)})\psi_\varepsilon$ for ε small enough. By Theorem 2 and Lemma 7 b) it holds in the norm of $\mathcal{L}\big(L^2(\mathcal{C}, d\mu_{\text{eff}}), \mathcal{D}(H_{\text{eff}}^\varepsilon)\big)$

$$
\begin{aligned}
\chi(H_{\text{eff}}^{(2)}) &= \tilde\chi^2(H_{\text{eff}}^{(2)})\,\chi(H_{\text{eff}}^{(2)}) \\
&= \tilde\chi^2(H_{\text{eff}}^\varepsilon)\,\chi(H_{\text{eff}}^{(2)}) + \mathcal{O}(\varepsilon^3) \\
&\overset{(68)}{=} U^\varepsilon \tilde\chi(H^\varepsilon)U^{\varepsilon*}\,\tilde\chi(H_{\text{eff}}^\varepsilon)\,\chi(H_{\text{eff}}^{(2)}) + \mathcal{O}(\varepsilon^3) \\
&= U^\varepsilon \tilde\chi(H^\varepsilon)U^{\varepsilon*}\,\chi(H_{\text{eff}}^{(2)}) + \mathcal{O}(\varepsilon^3).
\end{aligned}
$$

Therefore with $U^{\varepsilon*} = P^\varepsilon U^{\varepsilon*}$, $U^{\varepsilon*}U^\varepsilon = P^\varepsilon$, and $H_{\text{eff}}^\varepsilon = U^\varepsilon H^\varepsilon U^{\varepsilon*}$

$$
\begin{aligned}
H^\varepsilon\, U^{\varepsilon*}\psi_\varepsilon &= \big(P^\varepsilon + (1 - P^\varepsilon)\big)H^\varepsilon U^{\varepsilon*}\chi(H_{\text{eff}}^{(2)})\psi_\varepsilon \\
&= U^{\varepsilon*}H_{\text{eff}}^\varepsilon\chi(H_{\text{eff}}^{(2)})\psi_\varepsilon + (1 - P^\varepsilon)[H^\varepsilon, P^\varepsilon]\,U^{\varepsilon*}\chi(H_{\text{eff}}^{(2)})\psi_\varepsilon \\
&= U^{\varepsilon*}H_{\text{eff}}^{(2)}\psi_\varepsilon + (1 - P^\varepsilon)[H^\varepsilon, P^\varepsilon]\,\tilde\chi(H^\varepsilon)\,U^{\varepsilon*}\chi(H_{\text{eff}}^{(2)})\psi_\varepsilon \\
&\qquad\qquad\qquad\qquad\qquad\qquad + \mathcal{O}(\varepsilon^3\|\psi_\varepsilon\|_{\mathcal{H}_{\text{eff}}}) \\
&= E_\varepsilon\, U^{\varepsilon*}\psi_\varepsilon + \mathcal{O}(\varepsilon^3\|\psi_\varepsilon\|_{\mathcal{H}_{\text{eff}}}),
\end{aligned}
$$

where we made use of the assumption and Corollary 5 in the last step. This proves a) i) because $U^\varepsilon U^{\varepsilon*} = 1$ and thus $\|\psi_\varepsilon\|_{\mathcal{H}_{\text{eff}}} = \|U^{\varepsilon*}\psi_\varepsilon\|_{\overline{\mathcal{H}}}$.

To show a) ii) we now assume that we are given a family of eigenvalues (E_ε) of H^ε with $\limsup E_\varepsilon < E$ and a corresponding family of eigenfunctions (ψ^ε). Here this implies $\psi^\varepsilon = \chi(H^\varepsilon)\psi^\varepsilon$ for ε small enough. With $U^\varepsilon = U^\varepsilon P^\varepsilon$ and $U^{\varepsilon*}U^\varepsilon = P^\varepsilon$ we obtain

$$
\begin{aligned}
H_{\text{eff}}^{(2)}\, U^\varepsilon\psi^\varepsilon &= H_{\text{eff}}^{(2)}\, U^\varepsilon P^\varepsilon\,\tilde\chi(H^\varepsilon)\chi(H^\varepsilon)\psi^\varepsilon \\
&= H_{\text{eff}}^{(2)}\, U^\varepsilon\tilde\chi(H^\varepsilon)\,P^\varepsilon\chi(H^\varepsilon)\psi^\varepsilon + \mathcal{O}(\varepsilon^3) \\
&= H_{\text{eff}}^{(2)}\,\tilde\chi(H_{\text{eff}}^\varepsilon)\,U^\varepsilon\chi(H^\varepsilon)\psi^\varepsilon + \mathcal{O}(\varepsilon^3),
\end{aligned}
$$

where we used Lemma 7 a) & c) in the two last steps. In view of Theorem 2, we get

$$
\begin{aligned}
H_{\mathrm{eff}}^{(2)}\, U^\varepsilon \psi^\varepsilon &=& H_{\mathrm{eff}}^\varepsilon \tilde{\chi}(H_{\mathrm{eff}}^\varepsilon)\, U^\varepsilon \chi(H^\varepsilon)\psi^\varepsilon \,+\, \mathcal{O}(\varepsilon^3) \\
&=& U^\varepsilon H^\varepsilon U^{\varepsilon*}\, U^\varepsilon \tilde{\chi}(H^\varepsilon) P^\varepsilon \chi(H^\varepsilon)\psi^\varepsilon \,+\, \mathcal{O}(\varepsilon^3).
\end{aligned}
$$

Using again Lemma 7 a) & c) and the assumption we end up with

$$
\begin{aligned}
H_{\mathrm{eff}}^{(2)}\, U^\varepsilon \psi^\varepsilon &=& U^\varepsilon\, H^\varepsilon\, P^\varepsilon\, \chi(H^\varepsilon)\psi^\varepsilon \,+\, \mathcal{O}(\varepsilon^3) \;=\; U^\varepsilon\, H^\varepsilon \chi(H^\varepsilon)\psi^\varepsilon \,+\, \mathcal{O}(\varepsilon^3) \\
&=& E_\varepsilon\, U^\varepsilon \psi^\varepsilon \,+\, \mathcal{O}(\varepsilon^3).
\end{aligned}
$$

This finishes the proof of a) ii).

For b) we set $\psi_\varepsilon := D_\varepsilon^* M_\rho^* \psi^\varepsilon$ and observe that $-\varepsilon^2 \Delta_{\mathrm{v}} = D_\varepsilon \Delta_{\mathrm{v}} D_\varepsilon^*$ by Definition 1 and thus $-\varepsilon^2 M_\rho \Delta_{\mathrm{v}} M_\rho^* + V_0(q, \nu/\varepsilon) = M_\rho D_\varepsilon H_{\mathrm{f}} D_\varepsilon^* M_\rho^*$. Therefore the statement is equivalent to

$$
\limsup\, \langle \psi_\varepsilon | H_{\mathrm{f}} \psi_\varepsilon \rangle \,<\, \inf_{q \in \mathcal{C}} E_1 \|\psi_\varepsilon\|^2 \quad \Longrightarrow \quad \|U_\varepsilon \psi_\varepsilon\| \gtrsim \|\psi_\varepsilon\|
$$

because $U^\varepsilon := M_\rho^* U_\varepsilon D_\varepsilon^* M_\rho^*$ by definition in the proof of Theorem 1. We have

$$
\begin{aligned}
\langle \psi_\varepsilon | H_{\mathrm{f}} \psi_\varepsilon \rangle &=& \langle P_0 \psi_\varepsilon | H_{\mathrm{f}} P_0 \psi_\varepsilon \rangle \,+\, \langle (1 - P_0)\psi_\varepsilon | H_{\mathrm{f}}(1 - P_0)\psi_\varepsilon \rangle \\
&\geq& \inf_{q \in \mathcal{C}} E_{\mathrm{f}} \, \|P_0 \psi_\varepsilon\|^2 \,+\, \inf_{q \in \mathcal{C}} E_1 \, \|(1 - P_0)\psi_\varepsilon\|^2 \\
&=& \inf_{q \in \mathcal{C}} E_{\mathrm{f}} \, \|\psi_\varepsilon\|^2 \,+\, (\inf_{q \in \mathcal{C}} E_1 - \inf_{q \in \mathcal{C}} E_{\mathrm{f}}) \, \|(1 - P_0)\psi_\varepsilon\|^2 \\
&=& \inf_{q \in \mathcal{C}} E_{\mathrm{f}} \, \|\psi_\varepsilon\|^2 \,+\, (\inf_{q \in \mathcal{C}} E_1 - \inf_{q \in \mathcal{C}} E_{\mathrm{f}}) \, \|(1 - P_\varepsilon)\psi_\varepsilon\|^2 \,+\, \mathcal{O}(\varepsilon),
\end{aligned}
$$

where we used that $P_\varepsilon - P_0 = \mathcal{O}(\varepsilon)$ by Lemma 2 in the last step. Since E_{f} is a constraint energy band, hence, separated by a gap from E_1, and $\limsup \langle \psi_\varepsilon | H_{\mathrm{f}} \psi_\varepsilon \rangle < \inf_{q \in \mathcal{C}} E_1 \|\psi_\varepsilon\|^2$ by assumption, we may conclude that

$$
\limsup \|(1 - P_\varepsilon)\psi_\varepsilon\|^2 < \limsup \|\psi_\varepsilon\|^2.
$$

Because of $P_\varepsilon = U_\varepsilon^* U_\varepsilon$ this implies $\|U_\varepsilon \psi_\varepsilon\| \gtrsim \|\psi_\varepsilon\|$ for all ε small enough. $\quad\square$

4 The whole story

In Section 3 we proved our main theorems with the help of Lemmas 1 to 7. We still have to derive Lemmas 2 to 6, which is the task of this section. Before we can start with it, we have to carry out some technical preliminaries.

Remark 5 *Since $\mathcal{C}$ is of bounded geometry, it has a countable covering $(\Omega_j)_j$ of finite multiplicity (i.e. there is $l_0 \in \mathbb{N}$ such that each Ω_j overlaps with not more than l_0 of the others) by contractable geodesic balls of fixed diameter, and there is a corresponding partition of unity $(\xi_j \in C_0^\infty(\Omega_j))$ whose derivatives of any order are bounded uniformly in j (see e.g. App. 1 of [40]).*

We fix $j \in \mathbb{N}$. By geodesic coordinates with respect to the center $q \in \Omega_j$ we mean to choose an orthonormal basis $(v_i)_i$ of $T_q\mathcal{C}$ and to use the exponential mapping as a chart on Ω_j. Let $(x^i)_{i=1,\ldots,d}$ be geodesic coordinates on Ω_j. The bounded geometry of $\mathcal{C}$ that we assumed in (12) yields bounds uniform in j on the metric tensor g_{il} and its partial derivatives, thus, in particular, on all the inner curvatures of $\mathcal{C}$ and their partial derivatives. For the same reason the inverse of the metric tensor g_{il} is positive definite with a constant greater than zero uniform in j.

We choose an orthonormal basis of the normal space at the center of Ω_j and extend it radially to $N\mathcal{C}|_{\Omega_j} = N\Omega_j$ via the parallel transport by the normal connection $\nabla^\perp$ (defined in the appendix). In this way we obtain an orthonormal trivializing frame $(\nu_\alpha)_\alpha$ over Ω_j. Let $(n^\alpha)_{\alpha=1,\ldots,k}$ be bundle coordinates with respect to this frame. The connection coefficients $\Gamma_{i\alpha}^\gamma$ of the normal connection are given by $\nabla^\perp_{\partial_{x_i}} \nu_\alpha = \sum_{\gamma=1}^k \Gamma_{i\alpha}^\gamma \nu_\gamma$. Due to the smooth embedding of $\mathcal{C}$ assumed in (13) the exterior curvatures of $\mathcal{C}$, the curvature of $N\mathcal{C}$, as well as all their derivatives are globally bounded. This implies that all the partial derivatives of $\Gamma_{i\alpha}^\gamma$ and of the exterior curvatures of $\mathcal{C}$ are bounded uniformly in j in the coordinates $(x^i)_{i=1,\ldots,d}$ and $(n^\alpha)_{\alpha=1,\ldots,k}$.

From now on we implicitly sum over repeated indices. The vertical derivative in local coordinates is given by

$$(\nabla^{\mathrm{v}}_{\nu_\alpha} \psi)(x, n) \;=\; \partial_{n_\alpha} \psi(x, n). \tag{74}$$

and the horizontal connection is given by

$$(\nabla^{\mathrm{h}}_{\partial_{x_i}} \psi)(x, n) \;=\; \partial_{x^i} \psi(x, n) - \Gamma_{i\alpha}^\gamma \, n^\alpha \, \partial_{n^\gamma} \psi(x, n). \tag{75}$$

The former directly follows from the definition of ∇^{v} (see 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

$$(\nabla^\perp_{\partial_{x_i}} v)^\gamma \;=\; \partial_{x_i} n^\gamma + \Gamma_{i\alpha}^\gamma n^\alpha. \tag{76}$$

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

$$w(0) \;=\; x, \quad \dot{w}(0) \;=\; \partial_{x_i}, \quad \& \quad v(0) \;=\; n, \quad \nabla^\perp_{\dot{w}} v \;=\; 0.$$

Then by definition of ∇^{h} we have

$$
\begin{aligned}
(\nabla^{\mathrm{h}}_{\partial_{x_i}}\psi)(x,n) &= \tfrac{d}{ds}\big|_{s=0}\psi(w(s),v(s)) \\
&= \tfrac{d}{ds}\big|_{s=0}\psi(w(s),n) + \tfrac{d}{ds}\big|_{s=0}\psi(x,v(s)) \\
&= \partial_{x^i}\psi(x,n) + (\partial_{x^i}n^\gamma)\partial_{n^\gamma}\psi(x,n) \\
&= \partial_{x^i}\psi(x,n) - \Gamma^\gamma_{i\alpha}\,n^\alpha\,\partial_{n^\gamma}\psi(x,n),
\end{aligned}
$$

where we used (76) and the choice of the curve v in the last step.

With the formulas (74) and (75) it is easy to derive the properties of ∇^{h} that were stated in Lemma 4.

PROOF OF LEMMA 4 (SECTION 3.3):
Let $\tau,\tau_1,\tau_2 \in \Gamma(T\mathcal{C})$ and $\psi,\psi_1,\psi_2 \in C^2\big(\mathcal{C},\mathcal{H}_{\mathrm{f}}(q)\big)$. We fix a geodesic ball $\Omega \in \mathcal{C}$ and choose $(x^i)_{i=1,\dots,d}$ and $(n^\alpha)_{\alpha=1,\dots,k}$ as above. We first verify that ∇^{h} is metric, i.e. $\big(\mathrm{d}\,\langle\psi_1|\psi_2\rangle_{\mathcal{H}_{\mathrm{f}}}\big)(\tau) = \langle\nabla^{\mathrm{h}}_\tau\psi_1|\psi_2\rangle_{\mathcal{H}_{\mathrm{f}}} + \langle\psi_1|\nabla^{\mathrm{h}}_\tau\psi_2\rangle_{\mathcal{H}_{\mathrm{f}}}$. Since $\nabla^\perp$ is a metric connection, $\Gamma^\gamma_{i\alpha}$ is anti-symmetric in α and γ, in particular $\Gamma^\alpha_{i\alpha}=0$ for all α. Therefore an integration by parts yields that

$$
\big\langle\,\Gamma^\gamma_{i\alpha}n^\alpha\partial_{n^\gamma}\psi_1\,\big|\,\psi_2\,\big\rangle_{\mathcal{H}_{\mathrm{f}}} + \big\langle\,\psi_1\,\big|\,\Gamma^\gamma_{i\alpha}n^\alpha\partial_{n^\gamma}\psi_2\,\big\rangle_{\mathcal{H}_{\mathrm{f}}} = 0.
$$

Therefore we have

$$
\begin{aligned}
\big(\mathrm{d}\langle\psi_1|\psi_2\rangle\big)(\tau) &= \tau^i\langle\partial_{x_i}\psi_1|\psi_2\rangle + \tau^i\langle\psi_1|\partial_{x_i}\psi_2\rangle \\
&= \tau^i\big\langle(\partial_{x_i}-\Gamma^\gamma_{i\alpha}n^\alpha\partial_{n^\gamma})\psi_1|\psi_2\big\rangle + \tau^i\big\langle\psi_1|(\partial_{x_i}-\Gamma^\gamma_{i\alpha}n^\alpha\partial_{n^\gamma})\psi_2\big\rangle \\
&= \langle\nabla^{\mathrm{h}}_\tau\psi_1|\psi_2\rangle + \langle\psi_1|\nabla^{\mathrm{h}}_\tau\psi_2\rangle.
\end{aligned}
$$

To compute the curvature we notice that

$$
\begin{aligned}
\mathrm{R}^{\mathrm{h}}(\tau_1,\tau_2)\psi &= \big(\nabla^{\mathrm{h}}_{\tau_1}\nabla^{\mathrm{h}}_{\tau_2} - \nabla^{\mathrm{h}}_{\tau_2}\nabla^{\mathrm{h}}_{\tau_1} - \nabla^{\mathrm{h}}_{[\tau_1,\tau_2]}\big)\psi \\
&= \tau_1^i\tau_2^j\big(\nabla^{\mathrm{h}}_{\partial_{x_i}}\nabla^{\mathrm{h}}_{\partial_{x_j}} - \nabla^{\mathrm{h}}_{\partial_{x_j}}\nabla^{\mathrm{h}}_{\partial_{x_i}}\big)\psi \\
&= \tau_1^i\tau_2^j\Big((\partial_{x_i}\Gamma^\gamma_{j\alpha} - \partial_{x_j}\Gamma^\gamma_{i\alpha})n^\alpha\partial_{n^\gamma}\psi + \big[\Gamma^\delta_{i\alpha}n^\alpha\partial_{n^\delta},\Gamma^\gamma_{j\beta}n^\beta\partial_{n^\gamma}\big]\psi\Big).
\end{aligned}
$$

Using the commutator identity

$$
\big[\Gamma^\delta_{i\alpha}n^\alpha\partial_{n^\delta},\Gamma^\gamma_{j\beta}n^\beta\partial_{n^\gamma}\big]\psi = \big(\Gamma^\beta_{i\alpha}\Gamma^\gamma_{j\beta} - \Gamma^\beta_{j\alpha}\Gamma^\gamma_{i\beta}\big)n^\alpha\partial_{n^\gamma}\psi
$$

we obtain that

$$
\begin{aligned}
\mathrm{R}^{\mathrm{h}}(\tau_1,\tau_2)\psi &= \tau_1^i\tau_2^j\big(\partial_{x_i}\Gamma^\gamma_{j\alpha} - \partial_{x_j}\Gamma^\gamma_{i\alpha} + \Gamma^\beta_{i\alpha}\Gamma^\gamma_{j\beta} - \Gamma^\beta_{j\alpha}\Gamma^\gamma_{i\beta}\big)n^\alpha\partial_{n^\gamma}\psi \\
&= \tau_1^i\tau_2^j\,\overline{R}^\gamma_{\alpha ij}n^\alpha\partial_{n^\gamma}\psi \\
&= -\nabla^{\mathrm{v}}_{\mathrm{R}^\perp(\tau_1,\tau_2)\nu}\psi,
\end{aligned}
$$

which was the claim. $\qquad\square$

4.1 Elliptic estimates for the Sasaki metric

In the following, we deduce important properties of differential operators related to the Sasaki metric defined in the introduction (see (16)), in particular we will provide a-priori estimates for the associated Laplacian.

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 1 *Let g^{S} be the Sasaki metric on $N\mathcal{C}$ defined in (16). Choose $\Omega \subset \mathcal{C}$ where the normal bundle $N\mathcal{C}$ is trivializable and an orthonormal frame $(\nu_\alpha)_\alpha$ of $N\mathcal{C}|_\Omega$. Define $\Gamma_{i\alpha}^\gamma$ by $\nabla^\perp_{\partial_{x_i}} \nu_\alpha = \Gamma_{i\alpha}^\gamma \nu_\gamma$. In the corresponding bundle coordinates the dual metric tensor $g_{\mathrm{S}} \in \mathcal{T}^2_0(TN\mathcal{C})$ for all $q \in \Omega$ is given by:*

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

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

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

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

The proof was carried out by Wittich in [44]. From this expression we deduce the form of the associated Laplacian.

Corollary 6 *The Laplace-Beltrami operator associated to g_{S} is*

$$
\Delta_{\mathrm{S}} = \Delta_{\mathrm{h}} + \Delta_{\mathrm{v}}.
$$

PROOF OF COROLLARY 6:
We set $\mu := \det g_{ij}$ and $\mu_{\mathrm{S}} := \det(g_{\mathrm{S}})_{ab}$. Since $(\nu_\alpha)_{\alpha=1}^k$ is an orthonormal frame, we have that $g_{(q,0)}(\nu\alpha, \nu_\beta) = \delta^{\alpha\beta}$. So (74) and (75) imply that

$$
\Delta_{\mathrm{v}} = \partial_{n^\alpha} \delta^{\alpha\beta} \partial_{n^\beta} \ \& \ \Delta_{\mathrm{h}} = \mu^{-1}\big(\partial_{x^i} - \Gamma_{i\alpha}^\gamma n^\alpha \partial_{n^\gamma}\big) \mu g^{ij}\big(\partial_{x^j} - \Gamma_{i\alpha}^\gamma n^\alpha \partial_{n^\gamma}\big). \quad (77)
$$

Now plugging the expression for g_{S}^{ab} and $\det g_{\mathrm{S}}^{ab}$ from Proposition 1 into the general formula $\Delta_{\mathrm{S}} = \sum_{a,b=1}^{d+k} (\mu_{\mathrm{S}})^{-1} \partial_a \, \mu_{\mathrm{S}} \, g_{\mathrm{S}}^{ab} \partial_b$ yields the claim. $\qquad\square$

Next we gather some useful properties of Δ_{v}, Δ_{h}, and ∇^{h}. We recall that in Definition 2 we introduced the unitary operator D_ε for the isotropic dilation of the fibers with ε.

Lemma 8 *Let $f \in C^2(\mathbb{R})$ and $\tau \in \Gamma(T\mathcal{C})$ be arbitrary. Fix $\lambda \in \mathbb{R}$. It holds*

i) $D_\varepsilon \Delta_\mathrm{v} D_\varepsilon^* = \varepsilon^2 \Delta_\mathrm{v}, \quad D_\varepsilon \Delta_\mathrm{h} D_\varepsilon^* = \Delta_\mathrm{h}, \quad D_\varepsilon V_\varepsilon D_\varepsilon^* = V^\varepsilon,$

ii) $[\nabla_\tau^\mathrm{h}, \Delta_\mathrm{v}] = 0, \quad [\Delta_\mathrm{h}, \Delta_\mathrm{v}] = 0, \quad [\nabla_\tau^\mathrm{h}, f(\langle \lambda \nu \rangle)] = 0,$

iii) $[\Delta_\mathrm{v}, f(\langle \lambda \nu \rangle)] = \lambda f'(\langle \lambda \nu \rangle)\left(\lambda \frac{k \langle \lambda \nu \rangle^2 - |\lambda \nu|^2}{\langle \lambda \nu \rangle^3} + \frac{2}{\langle \lambda \nu \rangle} \nabla_{\lambda \nu}^\mathrm{v}\right) + \lambda^2 f''(\langle \lambda \nu \rangle)\frac{|\lambda \nu|^2}{\langle \lambda \nu \rangle^2}.$

In the following, we write $A \prec B$ when A is operator-bounded by B with a constant independent of ε, i.e. if $\mathcal{D}(B) \subset \mathcal{D}(A)$ and $\|A\psi\| \lesssim \|B\psi\| + \|\psi\|$ for all $\psi \in \mathcal{D}(B)$. We will have to estimate multiple applications of ∇^v and ∇^h by powers of H_ε, which was defined as $H_\varepsilon := D_\varepsilon^* M_\rho^* H^\varepsilon M_\rho D_\varepsilon$ with $H^\varepsilon := -\varepsilon^2 \Delta_{N\mathcal{C}} + V^\varepsilon$. Essential for our analysis, especially for the proofs of Lemmas 2 & 6, are the following statements:

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

i) $H_\varepsilon^m \prec \left(-\varepsilon^2 \Delta_\mathrm{h} - \Delta_\mathrm{v} + V_\varepsilon\right)^m \prec H_\varepsilon^m,$

ii) $\left(-\Delta_\mathrm{v}\right)^m \left(-\varepsilon^2 \Delta_\mathrm{h}\right)^M \prec H_\varepsilon^{M+m},$

iii) $\lambda^{-1} \langle \lambda \nu \rangle^l [H_\varepsilon^{M+1}, \langle \lambda \nu \rangle^{-l}] \prec H_\varepsilon^{M+1}$ *with a constant independent of λ,*

iv) $\langle \nu \rangle^{-4m_1 - 5m_2} (\nabla^\mathrm{v})^{m_1} (\varepsilon \nabla^\mathrm{h})^{m_2} \prec H_\varepsilon^m.$

The last three estimates rely on the following estimates in local coordinates. Here we a use covering $(\Omega_j)_j$ of $\mathcal{C}$ and coordinates $(x^i)_{i=1,\dots,d}$ and $(n^\alpha)_{\alpha=1,\dots,k}$ as in Remark 5 in the introduction to Section 4.

Lemma 10 *Let α, β, γ be multi-indices with $|\alpha| \leq 2l$, $|\alpha| + |\beta| \leq 2m$ and $|\gamma| = 2$. Set $\mu := \det g_{ij}$. For all smooth and compactly supported ψ it holds*

i) $\left(\sum_j \int_{\Omega_j} \int_{\mathbb{R}^k} |\partial_n^\alpha \psi|^2 \, dn \, \mu \, dx\right)^{1/2} \lesssim \|(-\Delta_\mathrm{v})^l \psi\| + \|\psi\|,$

ii) $\left(\sum_j \int_{\Omega_j} \int_{\mathbb{R}^k} |\partial_n^\gamma \psi|^2 \, dn \, \mu \, dx\right)^{1/2} \lesssim \|(-\varepsilon^2 \Delta_\mathrm{h} - \Delta_\mathrm{v})\psi\| + \|\psi\|,$

iii) $\left(\sum_j \int_{\Omega_j} \int_{\mathbb{R}^k} \langle \nu \rangle^{-8(|\alpha| + |\beta|)} |\partial_n^\alpha (\varepsilon^{|\beta|} \partial_x^\beta) \psi|^2 \, dn \, \mu \, dx\right)^{1/2}$
$$\lesssim \left\|\left(-\varepsilon^2 \Delta_\mathrm{h} - \Delta_\mathrm{v} + V_\varepsilon\right)^m \psi\right\| + \|\psi\|,$$

iv) $\left(\sum_j \int_{\Omega_j} \int_{\mathbb{R}^k} \langle \nu/\varepsilon \rangle^{-8(|\alpha| + |\beta|)} |\varepsilon^{|\alpha|} \partial_N^\alpha (\varepsilon^{|\beta|} \partial_x^\beta) \psi|^2 \, dN \, \mu \, dx\right)^{1/2}$
$$\lesssim \left\|\left(-\varepsilon^2 \Delta_\mathrm{h} - \varepsilon^2 \Delta_\mathrm{v} + V^\varepsilon\right)^m \psi\right\| + \|\psi\|.$$

We now provide the proofs of these three technical lemmas.

PROOF OF LEMMA 8:

We fix a geodesic ball $\Omega \subset \mathcal{C}$. Let $(\nu_\alpha)_{\alpha=1,\dots,k}$ be an orthonormal trivializing frame of $N\Omega$ with associated coordinates $(n^\alpha)_{\alpha=1,\dots,k}$ and $(x^i)_{i=1,\dots,d}$ be any coordinates on Ω. 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 (77).

Since $\nabla^\perp$ is a metric connection, $\Gamma_{i\alpha}^\gamma$ is anti-symmetric in α and γ and so (75) implies

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

Using that $\Delta_{\mathrm{v}} = \delta^{\alpha\beta} \partial_{n^\alpha} \partial_{n^\beta}$ by (77) we obtain that for any $\tau = \tau^i \partial_{x^i}$

$$[\nabla_\tau^{\mathrm{h}}, \Delta_{\mathrm{v}}] = \tau^i \Gamma_i^{\gamma\alpha} \left(\partial_{n^\alpha} \partial_{n^\gamma} - \partial_{n^\gamma} \partial_{n^\alpha} \right) = 0.$$

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

PROOF OF LEMMA 9:

We recall from Definition 2 that $V_\varepsilon = V_{\mathrm{c}} + D_\varepsilon^* W D_\varepsilon$ and that we assumed that V_{c} and W are in $C_{\mathrm{b}}^\infty \big(\mathcal{C}, C_{\mathrm{b}}^\infty(N_q \mathcal{C}) \big)$. These facts together imply that $V_\varepsilon \in C_{\mathrm{b}}^\infty \big(\mathcal{C}, C_{\mathrm{b}}^\infty(N_q \mathcal{C}) \big)$.

Since D_ε and M_ρ are unitary, Lemma 8 i) yields that Lemma 9 i) is equivalent to

$$(H^\varepsilon)^m \prec M_\rho \big(-\varepsilon^2 \Delta_{\mathrm{h}} - \varepsilon^2 \Delta_{\mathrm{v}} + V^\varepsilon \big)^m M_\rho^* \prec (H^\varepsilon)^m \tag{78}$$

for all $m \in \mathbb{N}$. By choice of $\overline{g}$ it coincides with the Sasaki metric g^{S} outside of $\mathcal{B}_\delta$ and, hence, so do Δ_{NC} and Δ_{S}. In addition, this means $\rho \equiv 1$ outside of $\mathcal{B}_\delta$ and so M_ρ is multiplication by 1 there. Then Corollary 6 implies $H^\varepsilon = M_\rho \big(-\varepsilon^2 \Delta_{\mathrm{h}} - \varepsilon^2 \Delta_{\mathrm{v}} + V^\varepsilon \big) M_\rho^*$ on $NC \setminus \mathcal{B}_\delta$. Hence, by introducing suitable cutoff functions it suffices to prove (78) for functions with support in $\mathcal{B}_{2\delta} \cap N\Omega_j$. The set $\mathcal{B}_{2\delta} \cap N\Omega_j$ is easily seen to be bounded with respect to both $\overline{g}$ and g^{S} and thus relatively compact because NC is complete with both $\overline{g}$ and g^{S} as explained in the sequel to the definition of g^{S} in (16). Furthermore, on $\mathcal{B}_{2\delta} \cap N\Omega_j$ both $(H^\varepsilon)^m$ and $M_\rho \big(-\varepsilon^2 \Delta_{\mathrm{h}} - \varepsilon^2 \Delta_{\mathrm{v}} + V^\varepsilon \big)^m M_\rho^*$ are elliptic operators with bounded coefficients of order $2m$. Therefore (78) follows from the usual elliptic estimates. These are uniform in j because $\mathcal{B}_{2\delta}$ is a subset of bounded geometry of NC with respect to both $\overline{g}$ and g^{S}, which was also explained in the sequel to (16).

In the following, we prove the estimates only on smooth and compactly supported functions, where we may apply Lemma 10. Then it is just a matter of

standard approximation arguments to extend them to the maximal domains of the operators on the right hand side of each estimate. In this context one should note that the mamixal domains $\mathcal{D}(H_\varepsilon^m)$ and $\mathcal{D}((-\varepsilon^2\Delta_{\mathrm{h}} - \Delta_{\mathrm{v}} + V_\varepsilon)^m)$ coincide for all $m \in \mathbb{N}$ by i).

We recall that $V_\varepsilon \in C_{\mathrm{b}}^\infty\big(\mathcal{C}, C_{\mathrm{b}}^\infty(N_q\mathcal{C})\big)$ and turn to ii). By i) we may replace H_ε by $-\varepsilon^2\Delta_{\mathrm{h}} - \Delta_{\mathrm{v}} + V_\varepsilon$. We first prove the statement for $M = 0$ inductively in m. In view of (77), Lemma 10 ii) implies that $-\Delta_{\mathrm{v}} \prec -\varepsilon^2\Delta_{\mathrm{h}} - \Delta_{\mathrm{v}}$ and thus also $-\varepsilon^2\Delta_{\mathrm{h}} \prec -\varepsilon^2\Delta_{\mathrm{h}} - \Delta_{\mathrm{v}}$. So due to the boundedness of V_ε the triangle inequality yields the statement for $m = 0$ as well as

$$- \varepsilon^2\Delta_{\mathrm{h}} \;\prec\; -\varepsilon^2\Delta_{\mathrm{h}} - \Delta_{\mathrm{v}} + V_\varepsilon. \tag{79}$$

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

Now we assume that the statement is true for some $m \in \mathbb{N}_0$. Since $V^\varepsilon \in C_{\mathrm{b}}^\infty$ and $N\mathcal{C}$ with the Sasaki metric g^{S} is complete, the operator $-\varepsilon^2\Delta_S + V_\varepsilon$ is self-adjoint on $\mathcal{H}$ and so is $-\varepsilon^2\Delta_{\mathrm{h}} - \Delta_{\mathrm{v}} + V_\varepsilon$, as it is unitary equivalent to $-\varepsilon^2\Delta_S + V^\varepsilon$ via D_ε. Therefore by the spectral calculus lower powers of $-\varepsilon^2\Delta_{\mathrm{h}} - \Delta_{\mathrm{v}} + V_\varepsilon$ 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

$$
\begin{aligned}
(-\Delta_{\mathrm{v}})^{m+1} \;\prec\;& (-\varepsilon^2\Delta_{\mathrm{h}} - \Delta_{\mathrm{v}} + V_\varepsilon)(-\Delta_{\mathrm{v}})^m \dotplus (-\Delta_{\mathrm{v}})^m \\
=\;& (-\Delta_{\mathrm{v}})^m(-\varepsilon^2\Delta_{\mathrm{h}} - \Delta_{\mathrm{v}} + V_\varepsilon) + \big[V_\varepsilon, (-\Delta_{\mathrm{v}})^m\big] \dotplus (-\Delta_{\mathrm{v}})^m \\
\prec\;& (-\varepsilon^2\Delta_{\mathrm{h}} - \Delta_{\mathrm{v}} + V_\varepsilon)^{m+1} \dotplus (-\Delta_{\mathrm{v}})^m \\
\prec\;& (-\varepsilon^2\Delta_{\mathrm{h}} - \Delta_{\mathrm{v}} + V_\varepsilon)^{m+1}.
\end{aligned}
$$

Here we used $V_\varepsilon \in C_{\mathrm{b}}^\infty(\mathcal{C}, C_{\mathrm{b}}^\infty(N_q\mathcal{C}))$, $\Delta_{\mathrm{v}} = \delta^{\alpha\beta}\partial_{n^\alpha}\partial_{n^\beta}$ locally, and i) of Lemma 10 to bound $\big[V_\varepsilon, (-\Delta_{\mathrm{v}})^m\big]$ by $(-\Delta_{\mathrm{v}})^m$. Using $[\Delta_{\mathrm{v}}, \Delta_{\mathrm{h}}] = 0$ and (79) we have

$$
\begin{aligned}
(-\Delta_{\mathrm{v}})^m(-\varepsilon^2\Delta_{\mathrm{h}}) \;=\;& (-\varepsilon^2\Delta_{\mathrm{h}})(-\Delta_{\mathrm{v}})^m \\
\prec\;& (-\varepsilon^2\Delta_{\mathrm{h}} - \Delta_{\mathrm{v}} + V)(-\Delta_{\mathrm{v}})^m \dotplus (-\Delta_{\mathrm{v}})^m.
\end{aligned}
$$

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

$$
\begin{aligned}
(-\Delta_{\mathrm{v}})^m(-\varepsilon^2\Delta_{\mathrm{h}})^2 \;=\;& (-\varepsilon^2\Delta_{\mathrm{h}})(-\Delta_{\mathrm{v}})^m(-\varepsilon^2\Delta_{\mathrm{h}}) \\
\prec\;& (-\varepsilon^2\Delta_{\mathrm{h}} - \Delta_{\mathrm{v}} + V_\varepsilon)(-\Delta_{\mathrm{v}})^m(-\varepsilon^2\Delta_{\mathrm{h}}) \\
& \dotplus (-\Delta_{\mathrm{v}})^m(-\varepsilon^2\Delta_{\mathrm{h}}) \\
\prec\;& (-\Delta_{\mathrm{v}})^m(-\varepsilon^2\Delta_{\mathrm{h}})(-\varepsilon^2\Delta_{\mathrm{h}} - \Delta_{\mathrm{v}} + V_\varepsilon) \\
& + \big[V_\varepsilon, (-\Delta_{\mathrm{v}})^m(-\varepsilon^2\Delta_{\mathrm{h}})\big] \dotplus (-\varepsilon^2\Delta_{\mathrm{h}} - \Delta_{\mathrm{v}} + V_\varepsilon)^{m+1} \\
\prec\;& (-\varepsilon^2\Delta_{\mathrm{h}} - \Delta_{\mathrm{v}} + V_\varepsilon)^{m+2} \dotplus \big[V_\varepsilon, (-\Delta_{\mathrm{v}})^m(-\varepsilon^2\Delta_{\mathrm{h}})\big],
\end{aligned}
$$

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where in the last step we used the statement for $M = 1$ and again that lower powers of $(-\varepsilon^2\Delta_h - \Delta_v + V_\varepsilon)$ are operator-bounded by higher powers. To handle the remaining term on the right hand side we choose a partition of unity $(\xi_j)_j$ corresponding to the covering $(\Omega_j)_j$ as in Remark 5 and orthonormal sections $(\tau_i^j)_{i=1,\dots,d}$ of $T\Omega_j$ for all j. Then it holds

$$\Delta_h = \sum_{j,i} \xi_j \nabla^h_{\tau_i^j, \tau_i^j} = \sum_{j,i} \xi_j (\nabla^h_{\tau_i^j} \nabla^h_{\tau_i^j} - \nabla^h_{\nabla_{\tau_i^j} \tau_i^j}). \tag{80}$$

The finite multiplicity of our coverings implies

$$\sum_{i,j} \int_{\Omega_j \times \mathbb{R}^k} \xi_j^2 \, \varepsilon\nabla^h_{\tau_i^j} \psi^* \, \varepsilon\nabla^h_{\tau_i^j} \psi \, d\mu \otimes d\nu \;\lesssim\; \int_{NC} g(\varepsilon\nabla^h \psi^*, \varepsilon\nabla^h \psi) d\mu \otimes d\nu$$

$$= \; \langle \psi | - \varepsilon^2\Delta_h \psi \rangle$$

$$\leq \; \| -\varepsilon^2\Delta_h \psi \| + \|\psi\|.$$

Therefore

$$\left[V_\varepsilon, (-\Delta_v)^m (-\varepsilon^2\Delta_h) \right] = \left[V_\varepsilon, (-\Delta_v)^m \right] (-\varepsilon^2\Delta_h) + (-\Delta_v)^m \left[V_\varepsilon, (-\varepsilon^2\Delta_h) \right]$$

$$\prec \; (-\Delta_v)^m(-\varepsilon^2\Delta_h) \dotplus \sum_{j,i} \xi_j (-\Delta_v)^m \varepsilon\nabla^h_{\tau_i^j} \dotplus (-\Delta_v)^m$$

$$= \; (-\varepsilon^2\Delta_h)(-\Delta_v)^m \dotplus \sum_{j,i} \xi_j \varepsilon\nabla^h_{\tau_i^j}(-\Delta_v)^m \dotplus (-\Delta_v)^m$$

$$\prec \; (-\varepsilon^2\Delta_h)(-\Delta_v)^m \dotplus (-\Delta_v)^m$$

$$\prec \; (-\varepsilon^2\Delta_h - \Delta_v + V_\varepsilon)^{m+2}.$$

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

$$\langle \lambda\nu \rangle^m \left[H_\varepsilon^3, \langle \lambda\nu \rangle^{-m} \right] = \langle \lambda\nu \rangle^m \left[H_\varepsilon, \langle \lambda\nu \rangle^{-m} \right] H_\varepsilon^2 + \langle \lambda\nu \rangle^m H_\varepsilon \left[H_\varepsilon, \langle \lambda\nu \rangle^{-m} \right] H_\varepsilon$$

$$+ \langle \lambda\nu \rangle^m H_\varepsilon^2 \left[H_\varepsilon, \langle \lambda\nu \rangle^{-m} \right].$$

We also only treat the hardest of these summands which is the last one. The arguments below also work for the other summands and for $M \in \{0, 1\}$. Inside of $\mathcal{B}_{2\delta}$ the estimate iii) can be reduced to standard elliptic estimates as in i). Therefore we may replace H_ε by $-\varepsilon^2\Delta_h - \Delta_v + V_\varepsilon$ because both operators coincide outside $\mathcal{B}_\delta$. In view of ii) of Lemma 8, we have

$$\lambda^{-1} \langle \lambda\nu \rangle^m \left(-\varepsilon^2\Delta_h - \Delta_v + V_\varepsilon \right)^2 \left[-\varepsilon^2\Delta_h - \Delta_v + V_\varepsilon, \langle \lambda\nu \rangle^{-m} \right]$$

$$= \; \lambda^{-1} \langle \lambda\nu \rangle^m \left(-\varepsilon^2\Delta_h - \Delta_v + V_\varepsilon \right)^2 \left[-\Delta_v, \langle \lambda\nu \rangle^{-m} \right]$$

$$= \; \Big(\langle \lambda\nu \rangle^m \left(-\Delta_v + V_\varepsilon \right)^2 \left[-\Delta_v, \langle \lambda\nu \rangle^{-m} \right] + \langle \lambda\nu \rangle^m \left[-\Delta_v, \langle \lambda\nu \rangle^{-m} \right] \left(-\varepsilon^2\Delta_h \right)^2$$

$$+ 2 \langle \lambda\nu \rangle^m \left(-\Delta_v + V_\varepsilon \right) \left[-\Delta_v, \langle \lambda\nu \rangle^{-m} \right] \left(-\varepsilon^2\Delta_h \right)$$

$$+ \langle \lambda\nu \rangle^m \left[-\varepsilon^2\Delta_h, V_\varepsilon \right] \left[-\Delta_v, \langle \lambda\nu \rangle^{-m} \right] \Big) \lambda^{-1}$$

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Because of $\Delta_{\mathrm{v}} = \delta^{\alpha\beta}\partial_{n_\alpha}\partial_{n_\beta}$ the operator $\langle\lambda\nu\rangle^m(-\Delta_{\mathrm{v}}+V_\varepsilon)^l\,[-\Delta_{\mathrm{v}},\langle\lambda\nu\rangle^{-m}]\lambda^{-1}$ contains only normal partial derivatives. It has coefficients bounded independently of λ for any l, as the commutator $[-\Delta_{\mathrm{v}},\langle\lambda\nu\rangle^{-m}]$ provides a λ due to Lemma 8 iii). So by i) of Lemma 10 it is bounded by $(-\Delta_{\mathrm{v}})^{l+1}$. Then ii) of Lemma 9 immediately allows to bound the first three terms by $(-\varepsilon^2\Delta_{\mathrm{h}}-\Delta_{\mathrm{v}}+V_\varepsilon)^3$. The last term can be treated as follows. In the proof of ii) we saw that $[-\varepsilon^2\Delta_{\mathrm{h}},V_\varepsilon]\prec-\varepsilon^2\Delta_{\mathrm{h}}$. Therefore

$$
\begin{aligned}
&\langle\lambda\nu\rangle^m\,[-\varepsilon^2\Delta_{\mathrm{h}},V_\varepsilon]\,[-\Delta_{\mathrm{v}},\langle\lambda\nu\rangle^{-m}]\lambda^{-1}\\
&\quad= \;[-\varepsilon^2\Delta_{\mathrm{h}},V_\varepsilon]\,\langle\lambda\nu\rangle^m\,[-\Delta_{\mathrm{v}},\langle\lambda\nu\rangle^{-m}]\,\lambda^{-1}\\
&\quad\prec\; -\varepsilon^2\Delta_{\mathrm{h}}\,\langle\lambda\nu\rangle^m\,[-\Delta_{\mathrm{v}},\langle\lambda\nu\rangle^{-m}]\,\lambda^{-1}\;\dotplus\;\langle\lambda\nu\rangle^m\,[-\Delta_{\mathrm{v}},\langle\lambda\nu\rangle^{-m}]\,\lambda^{-1}\\
&\quad=\; \langle\lambda\nu\rangle^m\,[-\Delta_{\mathrm{v}},\langle\lambda\nu\rangle^{-m}]\,\lambda^{-1}\,(-\varepsilon^2\Delta_{\mathrm{h}})\;\dotplus\;\langle\lambda\nu\rangle^m\,[-\Delta_{\mathrm{v}},\langle\lambda\nu\rangle^{-m}]\,\lambda^{-1}\\
&\quad\prec\; (-\Delta_{\mathrm{v}})\,(-\varepsilon^2\Delta_{\mathrm{h}})\;\dotplus\;(-\varepsilon^2\Delta_{\mathrm{h}})\;\dotplus\;(-\Delta_{\mathrm{v}})
\end{aligned}
$$

which is bounded independently of λ by $(-\varepsilon^2\Delta_{\mathrm{h}}-\Delta_{\mathrm{v}}+V_\varepsilon)^2$ again due to ii). Here again $[-\Delta_{\mathrm{v}},\langle\lambda\nu\rangle^{-m}]$ has provided the lacking λ.

In view of (74) and (75), the estimate iv) follows directly from i) of this lemma and iii) of Lemma 10. A polynomial weight is nescessary because here the unbounded geometry of $(N\mathcal{C},\overline{g})$ 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! $\qquad\square$

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 $\Delta_{\mathrm{v}} = \delta^{\alpha\beta}\partial_{n_\alpha}\partial_{n_\beta}$ is the Laplace operator on the fibers by (77) and that the measure $d\mu\otimes d\nu = dn\,\mu(x)dx$ is independent of n.

To deduce the second estimate we aim to show that

$$
\sum_{|\gamma|=2}\int_{\Omega_j}\int_{\mathbb{R}^k}|\,\partial_n^\gamma\Psi|^2\,dn\,\mu(x)dx \tag{81}
$$
$$
\lesssim\;\sum_{|\gamma|=2}\int_{\Omega_j}\int_{\mathbb{R}^k}|\,\partial_n^\gamma\Psi|\,\big(|(-\varepsilon^2\Delta_{\mathrm{h}}-\Delta_{\mathrm{v}})\Psi|+|\varepsilon\nabla^{\mathrm{h}}\psi|+|\Psi|\big)\,dn\,\mu(x)dx.
$$

with a constant independent of j. Then the claim follows from the Cauchy-Schwarz inequality and $\|\,|\varepsilon\nabla^{\mathrm{h}}\psi|\,\| = \langle\psi|-\varepsilon^2\Delta_{\mathrm{h}}\psi\rangle^{\frac12}\leq\langle\psi|(-\varepsilon^2\Delta_{\mathrm{h}}-\Delta_{\mathrm{v}})\psi\rangle^{\frac12}$ which is smaller than $\|(-\varepsilon^2\Delta_{\mathrm{h}}-\Delta_{\mathrm{v}})\Psi\|+\|\Psi\|$. We note that here and in the sequel there is no problem to sum up over j because the covering $(\Omega_j)_j$ has finite multiplicity!

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

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

On the other hand,

$$
\begin{aligned}
0 &\leq \int_{\Omega_j} \int_{\mathbb{R}^k} g\big(\varepsilon \nabla^{\mathrm{h}} \partial_{n^\beta} \psi^*, \varepsilon \nabla^{\mathrm{h}} \partial_{n^\beta} \psi\big) \, dn \, \mu(x) dx \\
&\overset{(75)}{=} \int_{\Omega_j} \int_{\mathbb{R}^k} g^{il} \varepsilon \big(\partial_{x^i} + \Gamma_{i\zeta}^\alpha n^\zeta \partial_{n^\alpha}\big) \partial_{n^\beta} \psi^* \, \varepsilon \big(\partial_{x^l} + \Gamma_{l\delta}^\eta n^\delta \partial_{n^\eta}\big) \partial_{n^\beta} \psi \, dn \, \mu(x) dx \\
&= \int_{\Omega_j} \int_{\mathbb{R}^k} -g^{il} \varepsilon \big(\partial_{x^i} + \Gamma_{i\zeta}^\alpha n^\zeta \partial_{n^\alpha}\big) \partial_{n^\beta} \partial_{n^\beta} \psi^* \, \varepsilon \big(\partial_{x^l} + \Gamma_{l\delta}^\eta n^\delta \partial_{n^\eta}\big) \psi \\
&\qquad\qquad - \varepsilon \, g^{il} \varepsilon \big(\partial_{x^i} + \Gamma_{i\zeta}^\alpha n^\zeta \partial_{n^\alpha}\big) \partial_{n^\beta} \psi^* \, \Gamma_{l\beta}^\eta \partial_{n^\eta} \psi \\
&\qquad\qquad - \varepsilon \, g^{il} \Gamma_{i\beta}^\alpha \partial_{n^\alpha} \partial_{n^\beta} \psi^* \, \varepsilon \big(\partial_{x^l} + \Gamma_{l\delta}^\eta n^\delta \partial_{n^\eta}\big) \psi \, dn \, \mu(x) dx \\
&= \int_{\Omega_j} \int_{\mathbb{R}^k} \partial_{n^\beta} \partial_{n^\beta} \psi^* \, \varepsilon^2 \Delta_{\mathrm{h}} \psi \; + \; \varepsilon^2 g^{ij} \Gamma_{i\beta}^\alpha \partial_{n^\alpha} \psi^* \, \Gamma_{l\beta}^\eta \partial_{n^\eta} \psi \\
&\qquad\qquad - 2\varepsilon \operatorname{Im}\Big(g^{il} \Gamma_{i\beta}^\alpha \partial_{n^\alpha} \partial_{n^\beta} \psi^* \, \varepsilon \big(\partial_{x^l} + \Gamma_{l\delta}^\eta n^\delta \partial_{n^\eta}\big) \psi\Big) \, dn \, \mu(x) dx
\end{aligned}
$$

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 $(-\varepsilon^2 \Delta_{\mathrm{h}} - \Delta_{\mathrm{v}})$-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

$$\int_{\Omega_j} \int_{\mathbb{R}^k} 2 \operatorname{Im}\Big(g^{il} \Gamma_{i\beta}^{\alpha} \partial_{n^{\alpha}} \partial_{n^{\beta}} \psi^* \, \varepsilon \big(\partial_{x^l} + \Gamma_{l\delta}^{\eta} n^{\delta} \partial_{n^{\eta}}\big) \psi \Big) \, dn \, \mu(x) dx$$

$$\leq \quad 2 \sup |(g^{il})^{\frac{1}{2}} \Gamma_{i\beta}^{\alpha}| \sum_{|\gamma|=2} \int_{\Omega_j} \int_{\mathbb{R}^k} |\partial_{n^{\alpha}} \partial_{n^{\beta}} \psi| \, |\varepsilon \nabla^{\mathrm{h}} \psi| \, dn \, \mu(x) dx.$$

This yields (81) because g^{il} and $\Gamma_{i\beta}^{\alpha}$ can be bounded independently of j in our coordinates due to the bounded geometry and the smooth embedding of $\mathcal{C}$ assumed in (12) and (13) as explained in Remark 5.

To see that iii) is just a reformulation of iv), we replace n by $N = \varepsilon n$ in iii), put in $\psi = D_{\varepsilon}^* \widetilde{\psi}$, and use that $(-\varepsilon^2 \Delta_{\mathrm{h}} - \Delta_{\mathrm{v}} + V_{\varepsilon}) D_{\varepsilon}^* = D_{\varepsilon}^* (-\varepsilon^2 \Delta_{\mathrm{h}} - \varepsilon^2 \Delta_{\mathrm{v}} + V^{\varepsilon})$ by Lemma 8.

So we immediately turn to iv). We notice that the powers of ε on both sides match because 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 $\Delta_{\mathrm{S}} = \Delta_{\mathrm{h}} + \Delta_{\mathrm{v}}$. We will prove by induction that for all $m \in \mathbb{N}_0$

$$\Big(\sum_{|\alpha| \leq m+2} \int_{\Omega_j} \int_{\mathbb{R}^k} \langle \nu \rangle^{-8|\alpha|} |\partial^{\alpha} \psi|^2 \, dN \, \mu \, dx \Big)^{\frac{1}{2}}$$

$$\lesssim \Big(\sum_{|\beta| \leq m} \int_{\Omega_j} \int_{\mathbb{R}^k} \langle \nu \rangle^{-8|\beta|} |\partial^{\beta} (-\Delta_{\mathrm{S}} + V) \psi|^2 \, dN \, \mu \, dx \Big)^{\frac{1}{2}} + \|\psi\| \quad (82)$$

with a constant independent of j. Applying this estimate iteratively we obtain our claim because as explained before $-\Delta_{\mathrm{S}} + V$ is self-adjoint and thus $(-\Delta_{\mathrm{S}} + V)^l$ is operator-bounded by $(-\Delta_{\mathrm{S}} + V)^m$ for $l \leq m$ due to the spectral calculus.

Before we begin with the induction we notice that, in view of Proposition 1, g_{S}^{ab} is positive definite 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, the constant depends on $\sup \Gamma_{i\gamma}^{\beta}$ and the inverse constant of positive definiteness of g^{il}, which are both uniformly bounded in our coordinates again due to (12) and (13).

We start the induction with the case $m = 0$. For $|\alpha| = 0$ there is nothing to prove. Since $\mu = \det g_{ab}^{\mathrm{S}}$ by Proposition 1, it holds $\Delta_{\mathrm{S}} = \mu^{-1} \partial_a \, \mu \, g_{\mathrm{S}}^{ab} \, \partial_b$. So

for $|\alpha| = 1$ we have

$$\sum_{|\alpha|=1} \int_{\Omega_j} \int_{\mathbb{R}^k} \langle\nu\rangle^{-8} |\partial^\alpha \psi|^2 \, dN\mu \, dx \;\lesssim\; \int_{\Omega_j} \int_{\mathbb{R}^k} g_{\mathrm{S}}^{ab} \partial_a \psi^* \, \partial_b \psi \, dN \, \mu \, dx$$

$$= \; -\int_{\Omega_j} \int_{\mathbb{R}^k} \psi^* \mu^{-1} \partial_a \, \mu \, g_{\mathrm{S}}^{ab} \, \partial_b \psi \, dN\mu \, dx$$

$$= \; \int_{\Omega_j} \int_{\mathbb{R}^k} \psi^* \big((-\Delta_{\mathrm{S}} + V - V)\psi\big) dN\mu \, dx$$

$$\leq \; \|\psi\| \big(\|(-\Delta_{\mathrm{S}} + V)\psi\| + \sup |V| \, \|\psi\|\big)$$

$$\lesssim \; \|(-\Delta_{\mathrm{S}} + V)\psi\|^2 \;+\; \|\psi\|^2$$

$$\leq \; \big(\|(-\Delta_{\mathrm{S}} + V)\psi\| \;+\; \|\psi\|\big)^2. \qquad (83)$$

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

$$\sum_{|\alpha|=2} \int_{\Omega_j} \int_{\mathbb{R}^k} \langle\nu\rangle^{-16} |\partial^\alpha \psi|^2 \, dN\mu \, dx$$

$$\lesssim \; \sum_c \int_{\Omega_j} \int_{\mathbb{R}^k} \langle\nu\rangle^{-14} g_{\mathrm{S}}^{ab} \partial_a \partial_c \psi^* \, \partial_b \partial_c \psi \, dN\mu \, dx$$

$$= \; \sum_c \int_{\Omega_j} \int_{\mathbb{R}^k} -\langle\nu\rangle^{-14} g_{\mathrm{S}}^{ab} \partial_a \partial_c \partial_c \psi^* \, \partial_b \psi$$

$$\hspace{3cm} -\mu^{-1}\big(\partial_c \, \mu \langle\nu\rangle^{-14} g_{\mathrm{S}}^{ab}\big) \partial_a \partial_c \psi^* \, \partial_b \psi \, dN\mu \, dx$$

$$= \; \sum_c \int_{\Omega_j} \int_{\mathbb{R}^k} \langle\nu\rangle^{-14} \partial_c \partial_c \psi^* \, (\Delta_{\mathrm{S}} - V + V)\psi$$

$$\hspace{1.5cm} -\Big(\mu^{-1}\big(\partial_c \, \mu \langle\nu\rangle^{-14} g_{\mathrm{S}}^{ab}\big)\partial_a \partial_c \psi^* - \big(\partial_a \langle\nu\rangle^{-14}\big) g_{\mathrm{S}}^{ab} \partial_c \partial_c \psi^*\Big) \partial_b \psi \, dN\mu \, dx$$

$$\lesssim \; \sum_{|\alpha|=2} \int_{\Omega_j} \int_{\mathbb{R}^k} \langle\nu\rangle^{-8} |\partial^\alpha \psi| \Big(|(-\Delta_{\mathrm{S}} + V)\psi| + |V||\psi| + \langle\nu\rangle^{-4}|\partial_b \psi|\Big) dN\mu \, dx$$

which yields (82) via (83) when we apply the Cauchy-Schwarz inquality and devide both sides by the square root of the left-hand side. Here we used that both $\mu^{-1}\big(\partial_c \, \mu \langle\nu\rangle^{-14} g_{\mathrm{S}}^{ab}\big)$ and $\big(\partial_a \langle\nu\rangle^{-14}\big) g_{\mathrm{S}}^{ab}$ are bounded by $\langle\nu\rangle^{-12}$. This is due to the facts that the derivatives of μ are globally bounded due to the bounded geometry of $\mathcal{C}$, that g_{S}^{ab} and its derivatives are bounded by $\langle\nu\rangle^2$ due to Proposition 1, 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 (82) is true for some fixed $m \in \mathbb{N}_0$. Then it suffices to consider multi-indices α with $|\alpha| = m + 3$ to show the statement for $m + 1$.

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We have

$$\sum_{|\alpha|=m+3} \int_{\Omega_j} \int_{\mathbb{R}^k} \langle \nu \rangle^{-8|\alpha|} |\partial^\alpha \psi|^2 \, dN\mu \, dx$$

$$\lesssim \sum_{|\tilde\alpha|=m+2} \int_{\Omega_j} \int_{\mathbb{R}^k} \langle \nu \rangle^{-8|\tilde\alpha|-6} g_S^{ab} \partial_a \partial^{\tilde\alpha} \psi^* \, \partial_b \partial^{\tilde\alpha} \psi \, dN\mu \, dx$$

$$= \sum_{|\tilde\alpha|=m+2} \int_{\Omega_j} \int_{\mathbb{R}^k} \langle \nu \rangle^{-8|\tilde\alpha|-6} \partial^{\tilde\alpha} \psi^* (-\Delta_S) \partial^{\tilde\alpha} \psi$$

$$- \partial^{\tilde\alpha} \psi^* \, (\partial_a \langle \nu \rangle^{-8|\tilde\alpha|-6}) \, g_S^{ab} \partial_b \partial^{\tilde\alpha} \psi \, dN\mu \, dx$$

$$= \sum_{|\tilde\alpha|=m+2} \int_{\Omega_j} \int_{\mathbb{R}^k} \langle \nu \rangle^{-8|\tilde\alpha|-6} \partial^{\tilde\alpha} \psi^* \, \partial^{\tilde\alpha} (-\Delta_S) \psi$$

$$- \partial^{\tilde\alpha} \psi^* \left((\partial_a \langle \nu \rangle^{-8|\tilde\alpha|-6}) \, g_S^{ab} \partial_b \partial^{\tilde\alpha} \psi + \langle \nu \rangle^{-8|\alpha|-6} [\Delta_S, \partial^{\tilde\alpha}] \psi \right) dN\mu \, dx$$

$$\lesssim \sum_{|\alpha|=m+3} \sum_{|\beta|=m+1} \int_{\Omega_j} \int_{\mathbb{R}^k} \langle \nu \rangle^{-4|\alpha|} |\partial^\alpha \psi| \, \langle \nu \rangle^{-4|\beta|} |\partial^\beta (-\Delta_S) \psi| \, dN\mu \, dx$$

$$+ \sum_{|\alpha|=m+3} \sum_{|\tilde\alpha|=m+2} \int_{\Omega_j} \int_{\mathbb{R}^k} \langle \nu \rangle^{-4|\tilde\alpha|} |\partial^{\tilde\alpha} \psi| \, \langle \nu \rangle^{-4|\alpha|} |\partial^\alpha \psi| \, dN\mu \, dx,$$

where we used that $[\Delta_S, \partial^{\tilde\alpha}]$ includes no terms with more than $m+3$ partial derivatives and that its coefficients are bounded by $\langle \nu \rangle^2$ times a constant independent of ε. Using again the Cauchy-Schwarz inequality, deviding by the square root of the left hand side, and applying the induction assumption to the $\tilde\alpha$-term we are almost done with the proof of (82) for $m+1$. We only have to introduce V in the Laplace term. We recall that it follows from $V_c, W \in C_b^\infty(\mathcal{C}, C_b^\infty(N_q\mathcal{C}))$ that $V_\varepsilon \in C_b^\infty(\mathcal{C}, C_b^\infty(N_q\mathcal{C}))$. When we put it in and use the triangle inquality we are left with the following error term:

$$\sum_{|\beta|=m+1} \int_{\Omega_j} \int_{\mathbb{R}^k} \langle \nu \rangle^{-8|\beta|} |\partial^\beta V \psi|^2 \, dN \, \mu \, dx$$

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

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 first replace the tangential derivatives in ∂^α by ∇^h and afterwards the normal derivatives by ∇^v. In view of (74) and (75), this costs at most a factor $\langle \nu \rangle^{-1}$ for each derivative. $\qquad \square$

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 $(H_{\mathcal{A}}^{\varepsilon}A^* - A^*H^{\varepsilon})P^{\varepsilon}$ is in $\mathcal{L}(\mathcal{D}(H^{\varepsilon}), L^2(\mathcal{A}, d\tau))$ at all. For $A^*H^{\varepsilon}P^{\varepsilon}$ this immediately follows from ii) and Corollary 5. So we have to show that $H_{\mathcal{A}}^{\varepsilon}A^*P^{\varepsilon} \in \mathcal{L}(\mathcal{D}(H^{\varepsilon}), L^2(\mathcal{A}, d\tau))$. By Corollary 5 we have

$$\|H_{\mathcal{A}}^{\varepsilon}A^*P^{\varepsilon}\|_{\mathcal{L}(\mathcal{D}(H^{\varepsilon}), L^2(\mathcal{A}, d\tau))} \lesssim \|H_{\mathcal{A}}^{\varepsilon}A^*\langle \nu/\varepsilon\rangle^{-l}\|_{\mathcal{L}(\mathcal{D}(H^{\varepsilon}), L^2(\mathcal{A}, d\tau))}$$

for any $l \in \mathbb{N}$. Now we again fix one of the geodesic balls $\Omega_j \subset \mathcal{C}$ of a covering as in Remark 5 and choose geodesic coordinates $(x_j^i)_{i=1,\ldots,d}$ and bundle coordinates $(n_j^{\alpha})_{\alpha=1,\ldots,k}$ 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 and the metric $\overline{g}$. However, this is compensated by $\langle \nu/\varepsilon\rangle^{-l}$. Choosing l big enough allows us to apply Lemma 10 iii) to bound $H_{\mathcal{A}}^{\varepsilon}A^*\langle \nu/\varepsilon\rangle^{-l}$ by $-\varepsilon^2\Delta_{\mathrm{h}} - \varepsilon^2\Delta_{\mathrm{v}} + V^{\varepsilon}$. The proof of Lemma 9 i) also shows that $-\varepsilon^2\Delta_{\mathrm{h}} - \varepsilon^2\Delta_{\mathrm{v}} + V^{\varepsilon} \prec H^{\varepsilon}$. To sum up over j is once more no problem because the covering $(\Omega_j)_j$ has finite multiplicity. Hence, $H_{\mathcal{A}}^{\varepsilon}A^*P^{\varepsilon} \in \mathcal{L}(\mathcal{D}(H^{\varepsilon}), L^2(\mathcal{A}, d\tau))$. With the same arguments one also sees that $\|A^*\langle \nu/\varepsilon\rangle^3 A (H_{\mathcal{A}}^{\varepsilon}A^* - A^*H^{\varepsilon})P^{\varepsilon}\|_{\mathcal{L}(\mathcal{D}(H^{\varepsilon}), L^2(\mathcal{A}, d\tau))} \lesssim 1$.

Since $\overline{g}$ is by definition the pullback of G on $\mathcal{B}_{\delta/2}$, the operators $H_{\mathcal{A}}^{\varepsilon}A^*$ and A^*H^{ε} coincide on functions whose support is contained in $\mathcal{B}_{\delta/2}$. But outside of $\mathcal{B}_{\delta/2}$, i.e. for $|\nu| \geq \delta/2$, we have that

$$\langle \nu/\varepsilon\rangle^{-3} = \left(\sqrt{\varepsilon^2 + |\nu|^2}\,/\varepsilon\right)^{-3} \leq 8\,\varepsilon^3/\delta^3.$$

Hence, denotig by $\chi_{\mathcal{B}_{\delta/2}}^{\mathrm{c}}$ the characteristic function of $N\mathcal{C} \setminus \mathcal{B}_{\delta/2}$ we obtain that $\|\chi_{\mathcal{B}_{\delta/2}}^{\mathrm{c}}\langle \nu/\varepsilon\rangle^3\|_{\infty} \lesssim \varepsilon^3$. Using that $A^*\psi \equiv 0$ on $\mathcal{A} \setminus \mathcal{B}$ for all ψ and $AA^* = 1$ by ii) we may estimate

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

which was the claim. $\qquad\qquad\square$

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 $\overline{g}$ around $\mathcal{C}$ because the Laplace-Beltrami operator depends on it. The use of the expansion will be justified by the fast decay of functions from the relevant subspaces P_0 and P_ε in the fibers.

Proposition 2 *Let $\overline{g}$ be the metric on $N\mathcal{C}$ defined in (17). Choose $\Omega \subset \mathcal{C}$ where the normal bundle $N\mathcal{C}$ is trivializable and an orthonormal frame $(\nu_\alpha)_\alpha$ of $N\mathcal{C}|_\Omega$ as in Remark 5. In the corresponding bundle coordinates the inverse metric tensor $\overline{g} \in \mathcal{T}_0^2(N\mathcal{C})$ has the following expansion for all $q \in \Omega$:*

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

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

$$\begin{aligned}
A^{ij}(q,n) &= g^{ij}(q) + n^\alpha \left(\mathrm{W}_{\alpha l}^{\ i} g^{lj} + g^{il} \mathrm{W}_{\alpha j}^{\ l} \right)(q) \\
&\quad + n^\alpha n^\beta \left(3 \, \mathrm{W}_{\alpha m}^{\ i} g^{ml} \mathrm{W}_{\beta l}^{\ j} + \mathrm{R}^i_{\ \alpha}{}^j_{\ \beta} \right)(q), \\
B^{\gamma\delta}(q,n) &= \delta_{\gamma\delta} + \tfrac{1}{3} n^\alpha n^\beta \mathrm{R}^\gamma_{\ \alpha}{}^\delta_{\ \beta}(q), \\
C_i^\gamma(q,n) &= -n^\alpha \Gamma_{i\alpha}^\gamma(q) + \tfrac{2}{3} n^\alpha n^\beta \mathrm{R}^\gamma_{\ \alpha i \beta}(q).
\end{aligned}$$

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). The remainder term r_1 and all its derivatives are bounded by $|n|^3$ times a constant.

For the proof we refer to the recent work of Wittich [44]. He does not calculate the second correction to C but it is easily deducable from his proof. Furthermore, Wittich actually calculates the expansion of the pullback of G, which coincides with $\overline{g}$ only on $\mathcal{B}_{\delta/2}$. Then r_1 is only locally bounded by $|n|^3$. To see that the global bound is true for $\overline{g}$ we recall that outside of $\mathcal{B}_\delta$ it coincides with g_S, which was explicitly given in Proposition 1. Comparing the expressions for $\overline{g}$ and g_S we obtain a bound by $|n|^2$ which is bounded by $|n|^3$ times a constant for $|n| \geq \delta$.

In addition, we need to know the expansion of the extra potential occuring in Lemma 1, which is also provided in [44]:

Proposition 3 *For $\rho := d\overline{\mu}/d\sigma$ with $d\sigma = d\mu \otimes d\nu$ it holds*

$$\begin{aligned}
V_\rho(q,n) &= -\tfrac{1}{4} \overline{g}_{(q,0)}(\eta, \eta) + \tfrac{1}{2} \kappa(q) - \tfrac{1}{6} \left(\overline{\kappa} + \mathrm{tr}_\mathcal{C} \, \overline{\mathrm{Ric}} + \mathrm{tr}_\mathcal{C} \, \overline{\mathrm{R}} \right)(q) + r_2(q,n) \\
&=: V_\mathrm{geom}(q) + r_2(q,n),
\end{aligned}$$

where η is the mean curvature normal, $\kappa, \overline{\kappa}$ are the scalar curvatures of $\mathcal{C}$ and $\mathcal{A}$, $\mathrm{tr}_\mathcal{C} \, \overline{\mathrm{Ric}}, \mathrm{tr}_\mathcal{C} \, \overline{\mathrm{R}}$ are the partial traces with respect to $T_q\mathcal{C} \subset T_q\mathcal{A}$ of the Ricci and the Riemann tensor of $\mathcal{A}$ and r_2 is bounded by $|n|$ times a constant.

Again there is only a local bound on r_2 in [44]. In our setting the global bound follows immediately from the coincidence of $d\overline{\mu}$ and $d\sigma$ outside of $\mathcal{B}_\delta$, see (19). With these two inputs the proof of Lemma 5 is not difficult anymore.

PROOF OF LEMMA 5 (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 choose a covering of $\mathcal{C}$ of finite multiplicity and local coordinates as at the beginning of Section 4 and start by proving $\|H_j P\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon^{m+1}),\mathcal{H})} \lesssim 1$ for $j \in \{0,1,2\}$. Exploiting that all the coefficients in H_j are bounded and have bounded derivatives due to the bounded geometry of $\mathcal{A}$ and $\mathcal{C}$ and the bounded derivatives of the embedding of $\mathcal{C}$ assumed in (12) and (13) we have

$$
\begin{aligned}
\|H_j P\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon^{m+1}),\mathcal{H})} &\lesssim \|H_j\langle\nu\rangle^{-16}\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon),\mathcal{H})} \\
&\lesssim \sum_{|\alpha|+|\beta|\leq 2} \|\langle\nu\rangle^{-8(|\alpha|+|\beta|)}\partial_n^\alpha \varepsilon^{|\beta|}\partial_x^\beta\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon),\mathcal{H})} \\
&\lesssim \|H_\varepsilon\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon),\mathcal{H})} = 1,
\end{aligned}
\tag{84}
$$

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 and V^ε it holds

$$
\begin{aligned}
\langle\phi\,|\,H_\varepsilon\psi_P\rangle &= \langle\phi\,|\,D_\varepsilon M_\rho(-\varepsilon^2\Delta_{\overline{g}}+V^\varepsilon)M_\rho^* D_\varepsilon^*\psi_P\rangle \\
&= \langle\phi\,|\,D_\varepsilon M_\rho(-\varepsilon^2\Delta_{\overline{g}})M_\rho^* D_\varepsilon^*\psi_P\rangle + \langle\phi\,|\,(V_c + D_\varepsilon^* W D_\varepsilon)\psi_P\rangle.
\end{aligned}
\tag{85}
$$

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

$$
\begin{aligned}
&\langle\phi\,|\,(V_c + D_\varepsilon^* W D_\varepsilon)\psi_P\rangle \\
&= \langle\phi\,|\,\big(V_0 + \varepsilon(\nabla_.^v W)(q,0) + \frac{1}{2}\varepsilon^2(\nabla_{.,.}^v W)(q,0)\big)\psi_P\rangle + \mathcal{O}(\varepsilon^3).
\end{aligned}
\tag{86}
$$

The error estimate in Proposition 3 yields that $\|D_\varepsilon^* r_2 D_\varepsilon\langle\nu\rangle^{-1}\psi\| \lesssim \varepsilon\|\psi\|$ and thus $\|D_\varepsilon r_2 D_\varepsilon^*\psi_P\| \lesssim \varepsilon\|\psi\|$. So Lemma 1 and Proposition 3 imply that

$$
\begin{aligned}
&\langle\phi\,|\,D_\varepsilon M_\rho(-\varepsilon^2\Delta_{\overline{g}})M_\rho^* D_\varepsilon^*\psi_P\rangle \\
&= \int_\mathcal{C}\int_{N_q\mathcal{C}} \varepsilon^2\,\overline{g}\big(\mathrm{d}D_\varepsilon^*\phi^*, \mathrm{d}D_\varepsilon^*\psi_P\big)\,d\nu\,d\mu + \varepsilon^2\langle\phi|D_\varepsilon V_\rho D_\varepsilon^*\psi_P\rangle \\
&= \int_\mathcal{C}\int_{N_q\mathcal{C}} \varepsilon^2\,\overline{g}\big(\mathrm{d}D_\varepsilon^*\phi^*, \mathrm{d}D_\varepsilon^*\psi_P\big)\,d\nu\,d\mu + \varepsilon^2\langle\phi|V_{\mathrm{geom}}\psi_P\rangle + \mathcal{O}(\varepsilon^3),
\end{aligned}
\tag{87}
$$

where we used that V_{geom} does not depend on ν.

Next we fix one of the geodesic balls $\Omega \subset \mathcal{C}$ of our covering and insert the expansion for $\bar{g}$ from Proposition 2 into (87). Noting that $\partial_{x^i} D_\varepsilon^* = D_\varepsilon^* \partial_{x^i}$ and $\partial_{n^\alpha} D_\varepsilon^* = \varepsilon^{-1} D_\varepsilon^* \partial_{n^\alpha}$ we then obtain that

$$
\int_\Omega \int_{N_q \mathcal{C}} \varepsilon^2 \, \bar{g}\big(\mathrm{d} D_\varepsilon^* \phi^*, \mathrm{d} D_\varepsilon^* \psi_P\big)\, d\nu\, d\mu
$$
$$
= \int_\Omega \int_{\mathbb{R}^k} \varepsilon^2 \Big(\big(\partial_{x^i} + C_i^\alpha(q,n)\partial_{n^\alpha}\big) D_\varepsilon^* \phi^*\Big) A^{ij}(q,n) \big(\partial_{x^j} + C_j^\beta(q,n)\partial_{n^\beta}\big) D_\varepsilon^* \psi_P
$$
$$
+ \varepsilon^2 \big(\partial_{n^\alpha} D_\varepsilon^* \phi^*\big) B^{\alpha\beta}(q,n)\, \partial_{n^\beta} D_\varepsilon^* \psi_P \; dn\, d\mu \, + \, \mathcal{O}(\varepsilon^3)
$$
$$
= \int_\Omega \int_{\mathbb{R}^k} \Big(\big(\varepsilon\partial_{x^i} + C_i^\alpha(q,\varepsilon n)\partial_{n^\alpha}\big)\phi^*\Big) A^{ij}(q,\varepsilon n) \big(\varepsilon\partial_{x^j} + C_j^\beta(q,\varepsilon n)\partial_{n^\beta}\big)\psi_P
$$
$$
+ \big(\partial_{n^\alpha}\phi^*\big) B^{\alpha\beta}(q,\varepsilon n)\, \partial_{n^\beta}\psi + \phi^* V_\varepsilon(q,n)\psi_P \; dn\, d\mu \, + \, \mathcal{O}(\varepsilon^3) \quad (88)
$$

because the bound on r_1 from Proposition 2 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 (84). After gathering the terms from (85) to (88) and plugging in the expressions for A, B, and C from Proposition 2 the rest of the proof is just a matter of identfying ∇^{v} and ∇^{h} via (74) and (75). When we sum up over the whole covering, the error stays of order ε^3 because our covering has finite multiplicity and the bounds are uniform as explained in Remark 5. $\square$

4.3 Construction of the superadiabatic subspace

Let E_{f} be a constraint energy band. We search for $P_\varepsilon \in \mathcal{L}(\mathcal{H})$ 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 an orthogonal projection, while the latter says that $P_\varepsilon \chi(H_\varepsilon)\mathcal{H}$ is invariant under the Hamiltonian H_ε up to errors of order ε^3.

Since the projector P_0 associated to E_{f} is a spectral projection of H_{f}, we know that $[H_{\mathrm{f}}, P_0] = 0$, $[E_{\mathrm{f}}, P_0] = 0$, and $H_{\mathrm{f}} P_0 = E_{\mathrm{f}} P_0$. Lemma 5 yields that $H_\varepsilon = H_0 + \mathcal{O}(\varepsilon)$ with $H_0 = -\varepsilon^2 \Delta_{\mathrm{h}} + H_{\mathrm{f}}$. So P_0 satisfies, at least formally, $[H_\varepsilon, P_0]\, \chi(H_\varepsilon) = [-\varepsilon^2 \Delta_{\mathrm{h}}, P_0]\, \chi(H_\varepsilon) + \mathcal{O}(\varepsilon) = \mathcal{O}(\varepsilon)$. Therefore 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 ignoring 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 $T_1 : \mathcal{H} \to \mathcal{H}$

to be determined. Assuming that $[P_1, -\varepsilon^2 \Delta_{\mathrm{h}} + E_{\mathrm{f}}] = \mathcal{O}(\varepsilon)$ we have

$$
\begin{aligned}
[H_\varepsilon, P_\varepsilon]/\varepsilon &= [H_0/\varepsilon + H_1, P_0 + \varepsilon P_1] + \mathcal{O}(\varepsilon) \\
&= [H_0/\varepsilon + H_1, P_0] + [H_0, P_1] + \mathcal{O}(\varepsilon) \\
&= [-\varepsilon \Delta_{\mathrm{h}} + H_1, P_0] + [H_{\mathrm{f}} - E_{\mathrm{f}}, P_1] + \mathcal{O}(\varepsilon) \\
&= [-\varepsilon \Delta_{\mathrm{h}} + H_1, P_0] + (H_{\mathrm{f}} - E_{\mathrm{f}}) T_1^* P_0 - P_0 T_1 (H_{\mathrm{f}} - E_{\mathrm{f}}) + \mathcal{O}(\varepsilon)
\end{aligned}
$$

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

$$
- \left(H_{\mathrm{f}} - E_{\mathrm{f}}\right)^{-1} (1 - P_0) \left([-\varepsilon \Delta_{\mathrm{h}}, P_0] + H_1\right) P_0 = (1 - P_0) T_1^* P_0 \qquad (89)
$$

and

$$
- P_0 \left([P_0, -\varepsilon \Delta_{\mathrm{h}}] + H_1\right) (1 - P_0) \left(H_{\mathrm{f}} - E_{\mathrm{f}}\right)^{-1} = P_0 T_1 (1 - P_0), \qquad (90)
$$

where we have used that the operator $H_{\mathrm{f}} - E_{\mathrm{f}}$ is invertible on $(1 - P_0)\mathcal{H}_{\mathrm{f}}$. In view of (89) and (90), we define T_1 by

$$
T_1 := - P_0 \left([P_0, -\varepsilon \Delta_{\mathrm{h}}] + H_1\right) R_{H_{\mathrm{f}}}(E_{\mathrm{f}}) + R_{H_{\mathrm{f}}}(E_{\mathrm{f}}) \left([-\varepsilon \Delta_{\mathrm{h}}, P_0] + H_1\right) P_0 \quad (91)
$$

with $R_{H_{\mathrm{f}}}(E_{\mathrm{f}}) = (1 - P_0)\left(H_{\mathrm{f}} - E_{\mathrm{f}}\right)^{-1}(1 - P_0)$. 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 condition i) for P_ε up to first order: Due to $P_0^2 = P_0$

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

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 $T_2 : \mathcal{H} \to \mathcal{H}$. The anti-symmetric part of T_2 is determined analogously with T_1 just by calculating the commutator $[P_\varepsilon, H_\varepsilon]$ up to second order and inverting $H_{\mathrm{f}} - E_{\mathrm{f}}$. One ends up with

$$
(T_2 - T_2^*)/2 = - P_0 \left([P^{(1)}, H^{(2)}]/\varepsilon^2\right) R_{H_{\mathrm{f}}}(E_{\mathrm{f}}) + R_{H_{\mathrm{f}}}(E_{\mathrm{f}}) \left([H^{(2)}, P^{(1)}]/\varepsilon^2\right) P_0
$$

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

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

which forces $T_2^* + T_2 = -T_1 T_1^*$ in order to satisfy condition i) upto second order.

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 Sordoni for the Born-Oppenheimer setting in [41] and by Tenuta and Teufel for a model of non-relativistic QED in [42].

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 $\operatorname{supp} \chi_{E+1} \subset (E_- - 2, E+2]$. Then we define

$$\tilde{P}_\varepsilon := P^{(2)} - P_0 = \varepsilon(T_1^* P_0 + P_0 T_1) + \varepsilon^2(T_1^* P_0 T_1 + T_2^* P_0 + P_0 T_2) \quad (92)$$

and

$$P_\varepsilon^{\chi_{E+1}} := P_0 + \tilde{P}_\varepsilon \chi_{E+1}(H_\varepsilon) + \chi_{E+1}(H_\varepsilon)\tilde{P}_\varepsilon\big(1 - \chi_{E+1}(H_\varepsilon)\big) \quad (93)$$

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 formula

$$P_\varepsilon := \frac{\mathrm{i}}{2\pi} \oint_\Gamma \big(P_\varepsilon^{\chi_{E+1}} - z\big)^{-1} dz, \quad (94)$$

where $\Gamma = \{z \in \mathbb{C} \,|\, |z - 1| = 1/2\}$ is the positively oriented circle around 1 (see e.g. [13]). Following here the construction of Nenciu and Sordoni [32] we define the unitary mapping $\tilde{U}_\varepsilon : P_\varepsilon\mathcal{H} \to P_0\mathcal{H}$ by the so-called Sz-Nagy formula:

$$\tilde{U}_\varepsilon := \big(P_0 P_\varepsilon + (1 - P_0)(1 - P_\varepsilon)\big)\big(1 - (P_\varepsilon - P_0)^2\big)^{-1/2}. \quad (95)$$

We now verify that P_ε and $\tilde{U}_\varepsilon$ have indeed all the properties which we stated in Lemmas 2 & 6 and state here again for convenience:

Proposition 4 *Fix $E < \infty$. Let E_f be a simple constraint energy band and $\chi_{E+1} \in C^\infty(\mathbb{R}, [0,1])$ with $\chi_{E+1}|_{(-\infty,E+1]} \equiv 1$ and $\operatorname{supp}\chi_{E+1} \subset (-\infty, E+2]$. For all ε small enough P_ε defined by (92)-(94) is a bounded operator on $\mathcal{H}$ and $\tilde{U}_\varepsilon$ defined by (95) 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 all $m \in \mathbb{N}_0$ and Borel function $\chi : \mathbb{R} \to [-1,1]$ with $\operatorname{supp}\chi \subset (-\infty, E+1]$ it holds $\|P_\varepsilon\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon^m))} \lesssim 1$ 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, it holds $E_{\mathrm{f}} \in C_{\mathrm{b}}^{\infty}(\mathcal{C})$, as well as:

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

ii) $\forall \, j, l \in \mathbb{N}_0: \, \|\langle\nu\rangle^l P_0 \langle\nu\rangle^j\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon))} \lesssim 1, \, \|[-\varepsilon^2 \Delta_{\mathrm{h}}, P_0]\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon), \mathcal{H})} \lesssim \varepsilon.$

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) $\|P_0 U_1^\varepsilon \langle\nu\rangle^l\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon^m))} \lesssim 1$ *for all $l \in \mathbb{N}_0$ and $m \in \{0,1\}$.*

v) *For $B_\varepsilon := P_0 \tilde{U}_\varepsilon \chi(H_\varepsilon)$ and all $u \in \{1, (U_1^\varepsilon)^*, (U_2^\varepsilon)^*\}$ it holds*

$$\left\| \, [-\varepsilon^2 \Delta_{\mathrm{h}} + E_{\mathrm{f}}, u P_0] B_\varepsilon \, \right\|_{\mathcal{L}(\mathcal{H})} = \mathcal{O}(\varepsilon).$$

vi) *For $R_{H_{\mathrm{f}}}(E_{\mathrm{f}}) := (1 - P_0)(H_{\mathrm{f}} - E_{\mathrm{f}})^{-1}(1 - P_0)$ it holds*

$$\left\| U_1^{\varepsilon *} B_\varepsilon + R_{H_{\mathrm{f}}}(E_{\mathrm{f}}) \left([-\varepsilon \Delta_{\mathrm{h}}, P_0] + H_1\right) P_0 B_\varepsilon \right\|_{\mathcal{L}(\mathcal{H}, \mathcal{D}(H_\varepsilon))} = \mathcal{O}(\varepsilon).$$

vii) *If $\varphi_{\mathrm{f}} \in C_{\mathrm{b}}^{\infty}(\mathcal{C}, \mathcal{H}_{\mathrm{f}})$, it holds*

$$\|U_0\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon), \mathcal{D}(-\varepsilon^2 \Delta_{\mathcal{C}} + E_{\mathrm{f}}))} \lesssim 1, \quad \|U_0^*\|_{\mathcal{L}(\mathcal{D}(-\varepsilon^2 \Delta_{\mathcal{C}} + E_{\mathrm{f}}), \mathcal{D}(H_\varepsilon))} \lesssim 1,$$

and there is $\lambda_0 \gtrsim 1$ with $\sup_q \|\mathrm{e}^{\lambda_0 \langle\nu\rangle} \varphi_{\mathrm{f}}(q)\|_{\mathcal{H}_{\mathrm{f}}(q)} \lesssim 1$ and

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

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

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

Lemma 11 *Let $V_0 \in C_b^{\infty}\big(\mathcal{C}, C_b^{\infty}(N\mathcal{C})\big)$ and E_{f} be a constraint energy band with family of projections P_0 as defined in Definition 3.*
Define $\nabla^{\mathrm{h}}_{\tau_1} P_0 := [\nabla^{\mathrm{h}}_{\tau_1}, P_0]$ and, inductively,

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

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 $\nabla^{\mathrm{v}}_{\nu_1, \dots, \nu_l} \nabla^{\mathrm{h}}_{\tau_1, \dots, \tau_m} P_0 := \big[\nabla^{\mathrm{v}}_{\nu_1}, \dots, [\nabla^{\mathrm{v}}_{\nu_l}, \nabla^{\mathrm{h}}_{\tau_1, \dots, \tau_m} P_0] \dots \big].$

i) Then $E_{\mathrm{f}} \in C_{\mathrm{b}}^{\infty}(\mathcal{C})$, $P_0 \in C_{\mathrm{b}}^{\infty}(\mathcal{C}, \mathcal{L}(\mathcal{H}_{\mathrm{f}}))$, and there is $\lambda_0 > 0$ independent of ε such that for all $\lambda \in [-\lambda_0, \lambda_0]$

$$\| \mathrm{e}^{\lambda\langle\nu\rangle} R_{H_{\mathrm{f}}}(E_{\mathrm{f}}) \mathrm{e}^{-\lambda\langle\nu\rangle} \|_{\mathcal{L}(\mathcal{H})} \lesssim 1$$

and

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

for all $\nu_1, \ldots, \nu_l \in \Gamma_{\mathrm{b}}(N\mathcal{C})$ and $\tau_1, \ldots, \tau_m \in \Gamma_{\mathrm{b}}(T\mathcal{C})$.

Let E_{f} be simple and φ_{f} be a corresponding family of eigenfunctions.
ii) If $\varphi_{\mathrm{f}} \in C_{\mathrm{b}}^{m}(\mathcal{C}, \mathcal{H}_{\mathrm{f}})$, then $\varphi_{\mathrm{f}} \in C_{\mathrm{b}}^{m}(\mathcal{C}, C_{b}^{\infty}(N\mathcal{C}))$. Furthermore,

$$\sup_{q \in \mathcal{C}} \| \mathrm{e}^{\lambda_0\langle\nu\rangle} \varphi_{\mathrm{f}}(q) \|_{\mathcal{H}_{\mathrm{f}}(q)} \lesssim 1, \quad \sup_{q \in \mathcal{C}} \| \mathrm{e}^{\lambda_0\langle\nu\rangle} \nabla^{\mathrm{v}}_{\nu_1,\ldots,\nu_l} \nabla^{\mathrm{h}}_{\tau_1,\ldots,\tau_m} \varphi_{\mathrm{f}}(q) \|_{\mathcal{H}_{\mathrm{f}}(q)} \lesssim 1$$

for all $\nu_1, \ldots, \nu_l \in \Gamma_{\mathrm{b}}(N\mathcal{C})$ and $\tau_1, \ldots, \tau_m \in \Gamma_{\mathrm{b}}(T\mathcal{C})$.
iii) If $\mathcal{C}$ is compact or contractable or if $E_{\mathrm{f}}(q) = \inf \sigma\big(H_{\mathrm{f}}(q)\big)$ for all $q \in \mathcal{C}$, then φ_{f} can be chosen such that $\varphi_{\mathrm{f}} \in C_{\mathrm{b}}^{\infty}(\mathcal{C}, \mathcal{H}_{\mathrm{f}})$.

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. We 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 12 *Let $\chi \in C_0^{\infty}(\mathbb{R})$ be non-negative and $\big(H, \mathcal{D}(H)\big)$ be self-adjoint on $\mathcal{H}$. Assume that there are $l \in \mathbb{Z}, m \in \mathbb{N}$ and $C_1 < \infty$ such that*

$$\|\langle\lambda\nu\rangle^{l} [H^{j}, \langle\lambda\nu\rangle^{-l}]\|_{\mathcal{L}(\mathcal{D}(H^m), \mathcal{H})} \leq C_1 \lambda \tag{96}$$

for all $\lambda \in (0, 1]$ and $1 \leq j \leq m$. Then there is $C_2 < \infty$ independent of H such that

$$\|\langle\nu\rangle^{l} \chi(H) \langle\nu\rangle^{-l}\|_{\mathcal{L}(\mathcal{H}, \mathcal{D}(H^m))} \leq C_1^{l} C_2.$$

This lemma can be applied to H_{ε} for $m \leq 3$ in view of Lemma 9. Now we give the proof of the proposition. Afterwards we take care of the two technical lemmas.

PROOF OF PROPOSITION 4:
We recall that $\mathcal{D}(H_{\varepsilon}^{0}) := \mathcal{H}$ and $E_{-} := \inf \sigma(H_{\varepsilon})$. Let $\chi_E \in C_0^{\infty}(\mathbb{R}, [0, 1])$ with $\chi_E|_{[E_-, E]} \equiv 1$ and $\operatorname{supp} \chi_E \subset [E_- - 1, E + 1]$. 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. In the sequel, we drop all ε-subscripts except

those of H_ε and write $\chi, \chi_E,$ and χ_{E+1} for $\chi(H_\varepsilon), \chi_E(H_\varepsilon),$ and $\chi_{E+1}(H_\varepsilon)$ respectively.

The proof of the proposition will be devided into several steps. We will often need that an operator $A \in \mathcal{L}(\mathcal{H})$ is in $\mathcal{L}(\mathcal{D}(H_\varepsilon^l), \mathcal{D}(H_\varepsilon^m))$ 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 $l_1 + l_2 \leq 2l$ such that for all $j \in \mathbb{N}_0$

$$(-\varepsilon^2\Delta_{\mathrm{h}} - \Delta_{\mathrm{v}} + V_\varepsilon)^m A \;\prec\; \langle\nu\rangle^{-j}(\nabla^{\mathrm{v}})^{l_1}(\varepsilon\nabla^{\mathrm{h}})^{l_2}. \tag{97}$$

Then we can use Lemma 9 to estimate:

$$
\begin{aligned}
\|H_\varepsilon^m A\psi\| + \|A\psi\| &\lesssim \|(-\varepsilon^2\Delta_{\mathrm{h}} - \Delta_{\mathrm{v}} + V_\varepsilon)^m A\psi\| + \|\psi\| \\
&\lesssim \|\langle\nu\rangle^{-4l_1-5l_2}(\nabla^{\mathrm{v}})^{l_1}(\varepsilon\nabla^{\mathrm{h}})^{l_2}\psi\| + \|\psi\| \\
&\lesssim \|H_\varepsilon^l\psi\| + \|\psi\|,
\end{aligned} \tag{98}
$$

which yields the desired bound.

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

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

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

Let λ_0 be as given by Lemma 11. When we choose a partition of unity $(\xi_j)_j$ corresponding to the covering $(\Omega_j)_j$ as in Remark 5 at the beginning of Section 4 and orthonormal sections $(\nu_\alpha^j)_{\alpha=1,\ldots,k}$ of $N\Omega_j$ and $(\tau_i^j)_{i=1,\ldots,d}$ of $T\Omega_j$ for all j, the coordinate formulas (77) imply

$$\Delta_{\mathrm{v}} = \sum_{j,\alpha} \xi_j \,\nabla_{\nu_\alpha^j}^{\mathrm{v}} \nabla_{\nu_\alpha^j}^{\mathrm{v}}, \quad \Delta_{\mathrm{h}} = \sum_{j,i} \xi_j(\nabla_{\tau_i^j}^{\mathrm{h}}\nabla_{\tau_i^j}^{\mathrm{h}} - \nabla_{\nabla_{\tau_i^j}\tau_i^j}^{\mathrm{h}}). \tag{99}$$

In order to obtain the estimate (97) for $A = \mathrm{e}^{\lambda_0\langle\nu\rangle} P_0 \,\mathrm{e}^{\lambda_0\langle\nu\rangle}$ we first commute all horizontal derivatives to the right and then the vertical ones. Using $V_0 \in C_b^\infty\big(\mathcal{C}, C_b^\infty(N\mathcal{C})\big)$ and Lemma 8 we end up with terms of the form $\xi_j\,\mathrm{e}^{\lambda\langle\nu\rangle}\big(\nabla_{\nu_1^j,\ldots,\nu_{l_3}^j}^{\mathrm{v}} \nabla_{\tau_1^j,\ldots,\tau_{l_4}^j}^{\mathrm{h}} P_0\big)\mathrm{e}^{\lambda\langle\nu\rangle}(\nabla^{\mathrm{v}})^{l_1}(\varepsilon\nabla^{\mathrm{h}})^{l_2}$ times a bounded function with $l_1 + l_2 \leq 2m$. By Lemma 11 we have

$$\xi_j\,\mathrm{e}^{\lambda\langle\nu\rangle}\big(\nabla_{\nu_1^j,\ldots,\nu_{l_3}^j}^{\mathrm{v}} \nabla_{\tau_1^j,\ldots,\tau_{l_4}^j}^{\mathrm{h}} P_0\big)\mathrm{e}^{\lambda\langle\nu\rangle}(\nabla^{\mathrm{v}})^{l_1}(\varepsilon\nabla^{\mathrm{h}})^{l_2} \;\prec\; \mathrm{e}^{-(\lambda_0-\lambda)\langle\nu\rangle}(\nabla^{\mathrm{v}})^{l_1}(\varepsilon\nabla^{\mathrm{h}})^{l_2}$$

which implies (97) due to $\lambda < \lambda_0$. This yields the first claim of Step 1 via (98).

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

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

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

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

The last statement is an immediate consequence because by definition of $\tilde{P}$

$$\mathrm{e}^{\lambda\langle\nu\rangle}\tilde{P}\mathrm{e}^{\lambda\langle\nu\rangle} \;=\; \varepsilon\,\mathrm{e}^{\lambda\langle\nu\rangle}\Big((T_1^* P_0 + P_0 T_1) \,+\, \varepsilon(T_1^* P_0 P_0 T_1 + T_2^* P_0 + P_0 T_2)\Big)\mathrm{e}^{\lambda\langle\nu\rangle}.$$

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 (97) for $A = \mathrm{e}^{\lambda\langle\nu\rangle} T_1^* P_0\,\mathrm{e}^{\lambda\langle\nu\rangle}$ we again commute all derivatives in $(-\varepsilon^2\Delta_{\mathrm{h}} - \Delta_{\mathrm{v}} + V_\varepsilon)^m$ and $T_1^* P_0$ to the right. In view of (91), the definition of T_1, we have to compute the commutator of $R_{H_{\mathrm{f}}}(E_{\mathrm{f}})$ with ∇^{h} and ∇^{v}. For arbitrary $\tau \in \Gamma_{\mathrm{b}}(T\mathcal{C})$ it holds

$$\begin{aligned}
\big[\nabla_\tau^{\mathrm{h}}, R_{H_{\mathrm{f}}}(E_{\mathrm{f}})\big] \;=\; &-(\nabla_\tau^{\mathrm{h}} P_0) R_{H_{\mathrm{f}}}(E_{\mathrm{f}}) \,-\, R_{H_{\mathrm{f}}}(E_{\mathrm{f}})(\nabla_\tau^{\mathrm{h}} P_0) \\
&- R_{H_{\mathrm{f}}}(E_{\mathrm{f}})\big[\nabla_\tau^{\mathrm{h}}, H_{\mathrm{f}} - E_{\mathrm{f}}\big] R_{H_{\mathrm{f}}}(E_{\mathrm{f}}).
\end{aligned}$$

with $\big[\nabla_\tau^{\mathrm{h}}, H_{\mathrm{f}} - E_{\mathrm{f}}\big] = (\nabla_\tau^{\mathrm{h}} V_0 - \nabla_\tau E_{\mathrm{f}})$. The latter is bounded because of $V_0 \in C_b^\infty\big(\mathcal{C}, C_b^\infty(N_q\mathcal{C})\big)$ by assumption and $E_{\mathrm{f}} \in C_{\mathrm{b}}^\infty(\mathcal{C})$ by Lemma 11. 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 $\|\mathrm{e}^{\lambda\langle\nu\rangle} R_{H_{\mathrm{f}}}(E_{\mathrm{f}})\,\mathrm{e}^{-\lambda\langle\nu\rangle}\|_{\mathcal{L}(\mathcal{H})} \lesssim 1$ by Lemma 11 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*

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

We recall that $P^{\chi_{E+1}}$ was defined as

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

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, $\|\chi_{E+1}\|_{\mathcal{L}(\mathcal{H},\mathcal{D}(H_\varepsilon^m))} \lesssim 1$ for every $m \in \mathbb{N}_0$. So the estimate for $\widetilde{P}$ 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 $\chi_{E+1}\widetilde{P}$ is the adjoint of $\widetilde{P}\chi_{E+1}$ and thus also bounded. This finally implies the boundedness of the third term, which establishes $\|P^{\chi_{E+1}}\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon^m))} \lesssim 1$ for all $m \in \mathbb{N}_0$.

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

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

It is straight forward to see that $\|\langle\nu\rangle^j\mathrm{e}^{-\lambda_0\langle\nu\rangle}\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon^m))} \lesssim 1$ 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 12 that $\|\langle\nu\rangle^{-l}\chi_{E+1}\langle\nu\rangle^l\|_{\mathcal{L}(\mathcal{H},\mathcal{D}(H_\varepsilon^3))} \lesssim 1$ because H_ε satisfies the assumption of Lemma 12 due to Lemma 9 iii). So Step 2 implies the desired estimate for the second term. Then it also follows for the third term again by estimating it by the adjoint of the second one.

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

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

We again restrict to $T_1^*P_0$ because the other cases can be treated in quite a similar way.

We note that E_{f} commutes with all operators contained in $T_1^*P_0$ but $\varepsilon\nabla^{\mathrm{h}}$. Furthermore, $\|[\varepsilon\nabla_\tau^{\mathrm{h}}, E_{\mathrm{f}}]P_0\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon^m))} = \varepsilon\|(\nabla_\tau E_{\mathrm{f}})P_0\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon^m))} = \mathcal{O}(\varepsilon)$ for any $\tau \in \Gamma_{\mathrm{b}}(TC)$ by Lemma 11. With this $\|[T_1^*P_0, E_{\mathrm{f}}]\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon^{m+2}),\mathcal{D}(H_\varepsilon^m))} = \mathcal{O}(\varepsilon)$ is easily verified.

We will obtain the claim of Step 4 for $T_1^*P_0$, if we are able to deduce that $\|[T_1^*P_0, -\varepsilon^2\Delta_{\mathrm{h}}]\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon^{m+2}),\mathcal{D}(H_\varepsilon^m))} = \mathcal{O}(\varepsilon)$. Again we aim at proving (97) by commuting all derivatives to the right. In Step 1 and Step 2 we have already treated the commutators of $-\varepsilon^2\Delta_{\mathrm{h}}$ with P_0 an $R_{H_{\mathrm{f}}}(E_{\mathrm{f}})$. So it remains to discuss the commutator of $\varepsilon\nabla_\tau^{\mathrm{h}}$ and $-\varepsilon^2\Delta_{\mathrm{h}}$, which does not vanish in general! To do so we again fix a covering $(\Omega_j)_{j\in\mathbb{N}}$ of $\mathcal{C}$ and choose a partition of unity $(\xi_j)_j$ corresponding to the covering $(\Omega_j)_j$ as in Remark 5, as well as orthonormal sections $(\tau_i^j)_{i=1,\dots,d}$ of $T\Omega_j$ for all j.

Recalling from (99) that $\Delta_{\mathrm{h}} = \sum_{i=1}^{d} \xi_j(\nabla_{\tau_i^j}^{\mathrm{h}}\nabla_{\tau_i^j}^{\mathrm{h}} - \nabla_{\nabla_{\tau_i^j}\tau_i^j}^{\mathrm{h}})$ we have

$$
\begin{aligned}
[\varepsilon\nabla_\tau^{\mathrm{h}}, -\varepsilon^2\Delta_{\mathrm{h}}] &= -\sum_{j,i}\xi_j\,[\varepsilon\nabla_\tau^{\mathrm{h}}, \varepsilon^2(\nabla_{\tau_i^j}^{\mathrm{h}}\nabla_{\tau_i^j}^{\mathrm{h}} - \nabla_{\nabla_{\tau_i^j}\tau_i^j}^{\mathrm{h}})] \\
&= -\varepsilon^3\sum_{j,i}\xi_j\big([\nabla_\tau^{\mathrm{h}}, \nabla_{\tau_i^j}^{\mathrm{h}}]\,\nabla_{\tau_i^j}^{\mathrm{h}} + \nabla_{\tau_i^j}^{\mathrm{h}}\,[\nabla_\tau^{\mathrm{h}}, \nabla_{\tau_i^j}^{\mathrm{h}}] - [\nabla_\tau^{\mathrm{h}}, \nabla_{\nabla_{\tau_i^j}\tau_i^j}^{\mathrm{h}}])\big) \\
&= -\varepsilon^3\sum_{j,i}\xi_j\Big(\mathrm{R}^{\mathrm{h}}(\tau, \tau_i^j)\,\nabla_{\tau_i^j}^{\mathrm{h}} + \nabla_{[\tau, \tau_i^j]}^{\mathrm{h}}\nabla_{\tau_i^j}^{\mathrm{h}} \\
&\qquad\qquad\qquad + \nabla_{\tau_i^j}^{\mathrm{h}}\,\mathrm{R}^{\mathrm{h}}(\tau, \tau_i^j) + \nabla_{\tau_i^j}^{\mathrm{h}}\nabla_{[\tau, \tau_i^j]}^{\mathrm{h}} + [\nabla_\tau^{\mathrm{h}}, \nabla_{\nabla_{\tau_i^j}\tau_i^j}^{\mathrm{h}}]\Big).
\end{aligned}
$$

In view of the expression for R^{h} in Lemma 4, 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 (97) using the decay provided by P_0. The estimate is independent of Ω_j because $\mathrm{R}^\perp$ is globally bounded due to our assumption on the embedding of $\mathcal{C}$ in (13).

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 5 when deriving the stated estimates. The proof of Step 2 entails that $P^{\chi_{E+1}} - P_0$ is of order ε in $\mathcal{L}(\mathcal{D}(H_\varepsilon^m))$ for any $m \in \mathbb{N}_0$. Therefore

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

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

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

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

the formal discussion presented there 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 (97) and (98).

Step 6: For ε small enough P & U are well-defined, $P^2 = P$, and $U|_{P\mathcal{H}}$ is unitary. $\|P\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon^m))} \lesssim 1$ and $\|P - P_0\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon^m))} = \mathcal{O}(\varepsilon)$ for all $m \in \mathbb{N}_0$.

Since P_0 is a projector and $\|P^{\chi_{E+1}} - P_0\|_{\mathcal{L}(\mathcal{H})} = \mathcal{O}(\varepsilon)$ by the proof of Step 3, we have

$$\|(P^{\chi_{E+1}})^2 - P^{\chi_{E+1}}\|_{\mathcal{L}(\mathcal{H})} = \mathcal{O}(\varepsilon). \tag{100}$$

Now the spectral mapping theorem for bounded operators 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 $P := \frac{\mathrm{i}}{2\pi} \oint_\Gamma \left(P_\varepsilon^{\chi_{E+1}} - z\right)^{-1} dz$ is an operator on $\mathcal{H}$ bounded independent of ε for $\varepsilon < 1/2C$ and satisfies $P^2 = P$ by the spectral calculus (see e.g. [13]). By the spectral theorem $P = \chi_{[1-C\varepsilon, 1+C\varepsilon]}(P^{\chi_{E+1}})$ and so $\|P - P^{\chi_{E+1}}\|_{\mathcal{L}(\mathcal{H})} = \mathcal{O}(\varepsilon)$. With $\|P^{\chi_{E+1}} - P_0\|_{\mathcal{L}(\mathcal{H})} = \mathcal{O}(\varepsilon)$ this entails $\|P - P_0\|_{\mathcal{L}(\mathcal{H})} = \mathcal{O}(\varepsilon)$. Hence, $1 - (P - P_0)^2$ is strictly positive and thus has a bounded inverse. Therefore $U := \left(P_0 P + (1 - P_0)(1 - P)\right)\left(1 - (P - P_0)^2\right)^{-1/2}$ is also bounded independent of ε as an operator on $\mathcal{H}$ and satisfies

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

We set $S := \left(1 - (P - P_0)^2\right)^{-1/2}$. 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 (100) 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 $\varepsilon < 1/2C$ and $z \in \partial B_{1/2}(1)$ the resolvent $\left(P^{\chi_{E+1}} - z\right)^{-1}$ is an operator bounded independent of ε even on $\mathcal{D}(H_\varepsilon^m)$. In view of P's definition, this implies $\|P\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon^m))} \lesssim 1$ for all $m \in \mathbb{N}$. Then we obtain that $\|P - P_0\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon^m))} = \mathcal{O}(\varepsilon)$ in the same way we did for $m = 0$.

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

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

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

$$
\begin{aligned}
[H_\varepsilon, P]\chi &= \frac{\mathrm{i}}{2\pi} \oint_\Gamma R_{P^{\chi_{E+1}}}(z)\, [H_\varepsilon, P^{\chi_{E+1}}]\, R_{P^{\chi_{E+1}}}(z)\, \chi_E\, \chi\, dz \\
&= \frac{\mathrm{i}}{2\pi} \oint_\Gamma R_{P^{\chi_{E+1}}}(z)\, [H_\varepsilon, P^{\chi_{E+1}}]\chi_E\, R_{P^{\chi_{E+1}}}(z)\, \chi \\
&\qquad + R_{P^{\chi_{E+1}}}(z)\, [H_\varepsilon, P^{\chi_{E+1}}]\big[R_{P^{\chi_{E+1}}}(z), \chi_E\big]\, \chi\, dz. \quad (101)
\end{aligned}
$$

Furthermore,

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

Since due to Step 5 we have $\left\|[P^{\chi_{E+1}}, H_\varepsilon]\right\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon^{m+1}),\mathcal{D}(H_\varepsilon^m))} = \mathcal{O}(\varepsilon)$ and $\left\|[P^{\chi_{E+1}}, H_\varepsilon]\chi_E\right\|_{\mathcal{L}(\mathcal{H},\mathcal{D}(H_\varepsilon^m))} = \mathcal{O}(\varepsilon^3)$, Lemma 7 yields

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

Applying these estimates, $\|R_{P^{\chi_{E+1}}}(z)\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon^m))} \lesssim 1$, and Step 5 to (101) we obtain $\|[H_\varepsilon, P]\chi(H_\varepsilon)\|_{\mathcal{L}(\mathcal{H},\mathcal{D}(H_\varepsilon^m))} = \mathcal{O}(\varepsilon^3)$.

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

This can be seen by applying the spectral calculus to $P^{\chi_{E+1}}$ which we know to be bounded and symmetric. Let $f : \mathbb{C} \to \mathbb{C}$ be defined by $f(z) := z$ and let $g : \mathbb{C} \to \{0, 1\}$ be the characteristic function of $B_{2/3}(1)$. Then due to (100) the spectral calculus implies that for ε small enough

$$
\begin{aligned}
P &= g(P^{\chi_{E+1}}) = f(P^{\chi_{E+1}})\, (g/f^2)(P^{\chi_{E+1}})\, f(P^{\chi_{E+1}}) \\
&= P^{\chi_{E+1}}\, (g/f^2)(P^{\chi_{E+1}})\, P^{\chi_{E+1}}. \quad (102)
\end{aligned}
$$

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

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

by the Cauchy integral formula for bounded operators (see e.g. [13]). In the proof of Step 6 we saw that $\|R_{P^{\chi_{E+1}}}(z)\|_{\mathcal{D}(H_\varepsilon)} \lesssim 1$ for $z \in \partial B_{1/2}(1)$, which implies that also $\|(g/f^2)(P^{\chi_{E+1}})\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon))} \lesssim 1$. Then applying the result of Step 3 to (102) yields the claim.

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

By construction we have $T_1 = -T_1^*$ and $T_2 + T_2^* = -T_1 T_1^*$ as well as $P_0 T_1 P_0 = 0$. With this it is straight forward to verify that $P^{(2)} = P_0 + \tilde{P}$ satisfies

$$\left\|\chi_E\big(P^{(2)}P^{(2)} - P^{(2)}\big)\chi\right\|_{\mathcal{L}(\mathcal{H},\mathcal{D}(H_\varepsilon^m))} = \mathcal{O}(\varepsilon^3). \tag{103}$$

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 7 yields

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

Recalling that $\|P^{\chi_{E+1}}\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon^m))} \lesssim 1$ due to Step 3 we have that in the norm of $\mathcal{L}(\mathcal{H}, \mathcal{D}(H_\varepsilon^m))$

$$
\begin{aligned}
\big((P^{\chi_{E+1}})^2 &- P^{\chi_{E+1}}\big)\chi \\
&= (P^{\chi_{E+1}} - 1)P^{\chi_{E+1}}\chi_E\chi \\
&= (P^{\chi_{E+1}} - 1)\chi_E P^{\chi_{E+1}}\chi + (P^{\chi_{E+1}} - 1)[P^{\chi_{E+1}}, \chi_E]\chi \\
&= \chi_E(P^{\chi_{E+1}} - 1)P^{\chi_{E+1}}\chi + [P^{\chi_{E+1}}, \chi_E]P^{\chi_{E+1}}\chi + \mathcal{O}(\varepsilon^3) \\
&= \chi_E(P^{(2)} - 1)P^{(2)}\chi + \mathcal{O}(\varepsilon^3) \\
&= \chi_E(P^{(2)}P^{(2)} - P^{(2)})\chi + \mathcal{O}(\varepsilon^3) \overset{(103)}{=} \mathcal{O}(\varepsilon^3).
\end{aligned}
$$

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

$$P - P^{\chi_{E+1}} = \frac{\mathrm{i}}{2\pi\mathrm{i}}\oint_\Gamma \frac{R_{P^{\chi_{E+1}}}(z) + R_{P^{\chi_{E+1}}}(1 - z)}{1 - z}\, dz\,\big((P^{\chi_{E+1}})^2 - P^{\chi_{E+1}}\big), \tag{104}$$

which was proved by Nenciu in [31], implies that

$$\left\|(P - P^{\chi_{E+1}})\chi(H_\varepsilon)\right\|_{\mathcal{L}(\mathcal{H},\mathcal{D}(H_\varepsilon^m))} = \mathcal{O}(\varepsilon^3). \tag{105}$$

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, $\|P_0 U_1 \langle \nu \rangle^l\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon^m))} \lesssim 1$ for all $l \in \mathbb{N}_0$ and $m \in \{0, 1\}$.

We define

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

and

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

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

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

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

$$\begin{aligned}
U_1 &= \varepsilon^{-1}\big(P_0\tilde{U}(1 - P_0) + (1 - P_0)\tilde{U}P_0\big) \\
&= \varepsilon^{-1}S\big(P_0 P(1 - P_0) + (1 - P_0)(1 - P)P_0\big) \\
&= \varepsilon^{-1}S\big(P_0(P - P_0)(1 - P_0) - (1 - P_0)(P - P_0)P_0\big). \quad (106)
\end{aligned}$$

By Taylor expansion it holds

$$1 - S = \int_0^1 \tfrac{1}{2}(1 - s)\big(1 - s(P - P_0)^2\big)^{-\frac{3}{2}} ds \, (P - P_0)^2. \quad (107)$$

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 $h(P - P_0) = \frac{\mathrm{i}}{2\pi}\oint_{\partial B_{1/2}(0)} h(z)R_{P-P_0}(z) \, dz$. This allows us to conclude that the integral on the right hand side of (107) 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

$$U_1 = \varepsilon^{-1}\big(P_0(P - P_0)(1 - P_0) - (1 - P_0)(P - P_0)P_0\big) + \mathcal{O}(\varepsilon). \quad (108)$$

This yields the desired bound because $\|P - P_0\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon^m))} = \mathcal{O}(\varepsilon)$. We now turn to the claim that $\|P_0 U_1\langle\nu\rangle^l\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon^m))} \lesssim 1$ for $m \in \{0, 1\}$: Using $[S, P_0] = 0$ and $\|P_0\langle\nu\rangle^l\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon^m))} \lesssim 1$ due to Step 1 we obtain from (106) that

$$\begin{aligned}
\|P_0 U_1\langle\nu\rangle^l\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon^m))} &= \|\varepsilon^{-1}SP_0(P - P_0)(1 - P_0)\langle\nu\rangle^l\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon^m))} \\
&\lesssim \|\varepsilon^{-1}(P - P_0)\langle\nu\rangle^l\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon^m))}
\end{aligned}$$

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 (104) 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 $B := P_0 \tilde{U} \chi(H_\varepsilon)$ and every $u \in \{1, U_1^*, U_2^*\}$

$$\left\| [-\varepsilon^2 \Delta_{\mathrm{h}} + E_{\mathrm{f}}, u P_0] B \right\|_{\mathcal{L}(\mathcal{H})} = \mathcal{O}(\varepsilon).$$

Again we restrict ourselves to the case $u = U_1^*$. It is obvious from the definition of U_1 in Step 10 that $[E_{\mathrm{f}}, U_1^* P_0] = 0$. In view of (108), U_1 (and thus also U_1^*) contains, up to terms of order ε, a factor $P - P_0$. As long as we commute $(-\varepsilon^2 \Delta_{\mathrm{h}}) P_0$ with the other factors, $P - P_0$ cancels the ε^{-1} in the definition of U_1 and the commutation yields the desired ε by Step 1. Using that $B = P_0 \tilde{U} \chi = P_0 \chi + \mathcal{O}(\varepsilon)$ we have

$$
\begin{aligned}
[-\varepsilon^2 \Delta_{\mathrm{h}}, U_1^* P_0] B \;&=\; [-\varepsilon^2 \Delta_{\mathrm{h}}, U_1^* P_0] P_0 \chi \;+\; \mathcal{O}(\varepsilon) \\
&\overset{(108)}{=}\; [-\varepsilon^2 \Delta_{\mathrm{h}}, \varepsilon^{-1}(1 - P_0)(P - P_0) P_0] P_0 \chi \;+\; \mathcal{O}(\varepsilon) \\
&=\; (1 - P_0)[-\varepsilon^2 \Delta_{\mathrm{h}}, \varepsilon^{-1}(P - P_0)] P_0 \chi_E \chi \;+\; \mathcal{O}(\varepsilon) \\
&=\; (1 - P_0)[-\varepsilon^2 \Delta_{\mathrm{h}}, \varepsilon^{-1}(P - P_0)\chi_E] P_0 \chi \;+\; \mathcal{O}(\varepsilon),
\end{aligned}
$$

The last step follows from $[(-\varepsilon^2 \Delta_{\mathrm{h}}) P_0, \chi_E] \chi = \mathcal{O}(\varepsilon)$, which is implied by Lemma 7 because $(-\varepsilon^2 \Delta_{\mathrm{h}}) P_0$ satisfies the assumption on A in Lemma 5 and thus

$$
\begin{aligned}
[H_\varepsilon, (-\varepsilon^2 \Delta_{\mathrm{h}}) P_0] \chi \;&=\; [-\varepsilon^2 \Delta_{\mathrm{h}} + H_{\mathrm{f}}, (-\varepsilon^2 \Delta_{\mathrm{h}}) P_0] \chi \;+\; \mathcal{O}(\varepsilon) \\
&=\; [V_0, -\varepsilon^2 \Delta_{\mathrm{h}}] P_0 \chi \;-\; \varepsilon^2 \Delta_{\mathrm{h}} [-\varepsilon^2 \Delta_{\mathrm{h}}, P_0] \chi \;+\; \mathcal{O}(\varepsilon) \\
&=\; \mathcal{O}(\varepsilon)
\end{aligned}
$$

as in Step 1. Furthermore, due to Step 9

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

On the one hand,

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

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by Step 1 and Step 2. On the other hand,

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

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

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

All the following estimates will be in the norm of $\mathcal{L}\big(\mathcal{H}, \mathcal{D}(H_\varepsilon)\big)$. It is easy to prove $[P_0, \chi_E] \chi = \mathcal{O}(\varepsilon)$ in the same way we proved $[(-\varepsilon^2 \Delta_{\mathrm{h}}) P_0, \chi_E] \chi = \mathcal{O}(\varepsilon)$ in Step 10. Using again that $B = P_0 \tilde{U} \chi = P_0 \chi + \mathcal{O}(\varepsilon)$, $\chi = \chi_E \chi$, as well as $P - P_0 = \mathcal{O}(\varepsilon)$ we obtain that

$$
\begin{aligned}
U_1^* B &= U_1^* P_0 \chi_E \chi + \mathcal{O}(\varepsilon) \\
&\overset{(108)}{=} \varepsilon^{-1}(1 - P_0)(P - P_0) P_0 \chi_E \chi + \mathcal{O}(\varepsilon) \\
&= \varepsilon^{-1}(1 - P_0)(P - P_0) \chi_E P_0 \chi + \mathcal{O}(\varepsilon) \\
&\overset{(105)}{=} \varepsilon^{-1}(1 - P_0)(P^{\chi_E + 1} - P_0) \chi_E P_0 \chi + \mathcal{O}(\varepsilon) \\
&= (1 - P_0)\big(P_1 \chi_{E+1} + (1 - \chi_{E+1}) P_1 \chi_{E+1}\big) \chi_E P_0 \chi + \mathcal{O}(\varepsilon) \\
&= (1 - P_0)(T_1^* P_0 + P_0 T_1) \chi_E P_0 \chi + \mathcal{O}(\varepsilon) \\
&= (1 - P_0) T_1^* P_0 \chi + \mathcal{O}(\varepsilon) \\
&= T_1^* P_0 B + \mathcal{O}(\varepsilon)
\end{aligned}
$$

because $(1 - P_0) T_1^* P_0 = T_1^* P_0$ by definition and $P_0 \chi = B + \mathcal{O}(\varepsilon)$.

Step 13: It holds $E_{\mathrm{f}} \in C_{\mathrm{b}}^\infty(\mathcal{C})$. If $\varphi_{\mathrm{f}} \in C_{\mathrm{b}}^\infty(\mathcal{C}, \mathcal{H}_{\mathrm{f}})$, then

$$
\|U_0\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon), \mathcal{D}(-\varepsilon^2 \Delta_{\mathcal{C}} + E_{\mathrm{f}}))} \lesssim 1, \quad \|U_0^*\|_{\mathcal{L}(\mathcal{D}(-\varepsilon^2 \Delta_{\mathcal{C}} + E_{\mathrm{f}}), \mathcal{D}(H_\varepsilon))} \lesssim 1,
$$

and there is $\lambda_0 \gtrsim 1$ *with* $\sup_q \|\mathrm{e}^{\lambda_0 \langle \nu \rangle} \varphi_{\mathrm{f}}(q)\|_{\mathcal{H}_{\mathrm{f}}(q)} \lesssim 1$ *and*

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

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

We recall that $U_0 \psi = \langle \varphi_{\mathrm{f}} | \psi \rangle_{\mathcal{H}_{\mathrm{f}}}$ and $U_0^* \psi = \varphi_{\mathrm{f}} \psi$. Using Lemma 11 ii) we easily obtain $\|(-\varepsilon^2 \Delta_{\mathcal{C}} + E_{\mathrm{f}}) U_0 \psi\| \lesssim \|\mathrm{e}^{-\lambda_0 \langle \nu \rangle / 2} (\nabla^{\mathrm{h}})^2 \psi\|$ for all $\psi \in \mathcal{D}(H_\varepsilon)$

and $\|H^\varepsilon U_0^* \psi\| \lesssim \|\varepsilon^2 \nabla \mathrm{d}\psi\|$ for all $\psi \in \mathcal{D}(-\varepsilon^2 \Delta_{\mathcal{C}} + E_\mathrm{f})$. By (98) the former estimate implies $\|U_0\|_{\mathcal{L}(\mathcal{D}(H_\varepsilon), \mathcal{D}(-\varepsilon^2\Delta_{\mathcal{C}} + E_\mathrm{f}))} \lesssim 1$. Due to the bounded geometry of $\mathcal{C}$ any differential operator of second order with coefficients in C_b^∞ is operator-bounded by the elliptic $-\Delta_{\mathcal{C}}$. So the latter estimate implies $\|U_0^*\|_{\mathcal{L}(\mathcal{D}(-\varepsilon^2\Delta_{\mathcal{C}} + E_\mathrm{f}), \mathcal{D}(H_\varepsilon))} \lesssim 1$. The other statements are true by Lemma 11 i) and ii).

The results of Step 1 and Steps 6 to 13 together form Proposition 4. $\qquad\square$

PROOF OF LEMMA 11:
Because of $V_0 \in C_\mathrm{b}^\infty(\mathcal{C}, C_\mathrm{b}^\infty(N_q\mathcal{C}))$ and $[\nabla_\tau^\mathrm{h}, \Delta_\mathrm{v}] = 0$ for all τ due to Lemma 8 the mapping $q \mapsto (H_\mathrm{f}(q) - z)^{-1}$ is in $C_\mathrm{b}^\infty(\mathcal{C}, \mathcal{L}(\mathcal{H}_\mathrm{f}))$. Since E_f is a constraint energy band and thus separated, the projection $P_0(q)$ associated to $E_\mathrm{f}(q)$ is given via the Riesz formula:

$$P_0(q) \;=\; \frac{\mathrm{i}}{2\pi} \oint_{\gamma(q)} \big(H_\mathrm{f}(q) - z\big)^{-1} dz,$$

where $\gamma(q)$ is positively oriented closed curve encircling $E_\mathrm{f}(q)$ once. It can be chosen independent of $q \in \mathcal{C}$ locally because the gap condition is uniform. Therefore $(H_\mathrm{f}(\cdot) - z)^{-1} \in C_\mathrm{b}^\infty(\mathcal{C}, \mathcal{L}(\mathcal{H}_\mathrm{f}))$ entails $P_0 \in C_\mathrm{b}^\infty(\mathcal{C}, \mathcal{L}(\mathcal{H}_\mathrm{f}))$. This means in particular that $P_0 \mathcal{H}$ is a smooth subbundle. Therefore locally it is spanned by a smooth section φ_f of normalized eigenfunctions. By

$$E_\mathrm{f}(q) P_0(q) \;=\; H_\mathrm{f}(q) P_0(q) \;=\; \frac{\mathrm{i}}{2\pi} \oint_{\gamma(q)} z\big(H_\mathrm{f}(q) - z\big)^{-1} dz$$

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

$$
\begin{aligned}
\nabla_\tau \mathrm{tr}\big(E_\mathrm{f} P_0\big) \;&=\; \nabla_\tau \mathrm{tr}\big((E_\mathrm{f} P_0) P_0\big) \\
&=\; \mathrm{tr}\big((\nabla_\tau^\mathrm{h} E_\mathrm{f} P_0) P_0 \,+\, (E_\mathrm{f} P_0) \nabla_\tau^\mathrm{h} P_0\big) \\
&=\; \mathrm{tr}\big((\nabla_\tau^\mathrm{h} E_\mathrm{f} P_0) P_0\big) \,+\, \mathrm{tr}\big((E_\mathrm{f} P_0) \nabla_\tau^\mathrm{h} P_0\big) \;<\; \infty
\end{aligned}
$$

for all $\tau \in \Gamma_\mathrm{b}(T\mathcal{C})$ because P_0 and $E_\mathrm{f} P_0$ are trace-class operators and the product of a trace-class operator and a bounded operator is again a trace-class operator (see e.g. [35], Theorem VI.19). The argument that higher derivatives of $E_\mathrm{f} P_0$ are trace-class operators is very similar.

Next we will prove the statement about invariance of exponential decay under the application of $R_{H_\mathrm{f}}(E_\mathrm{f}) := (1 - P_0)(H_\mathrm{f} - E_\mathrm{f})^{-1}(1 - P_0)$. So let $\Psi \in \mathcal{H}_\mathrm{f}$ be

arbitrary. The claim is equivalent to showing that there is $\lambda_0 > 0$ such that for all $\lambda \in [-\lambda_0, \lambda_0]$

$$\Phi := \mathrm{e}^{\lambda \langle \nu \rangle} R_{H_{\mathrm{f}}}(E_{\mathrm{f}}) \mathrm{e}^{-\lambda \langle \nu \rangle} \Psi$$

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

$$\|\Phi\|_{\mathcal{H}} \lesssim \|\mathrm{e}^{\lambda \langle \nu \rangle}(H_{\mathrm{f}} - E_{\mathrm{f}}) \mathrm{e}^{-\lambda \langle \nu \rangle} \Phi\|_{\mathcal{H}} \tag{109}$$

because

$$
\begin{aligned}
\|\mathrm{e}^{\lambda \langle \nu \rangle}(H_{\mathrm{f}} - E_{\mathrm{f}}) \mathrm{e}^{-\lambda \langle \nu \rangle} \Phi\|_{\mathcal{H}} &= \|\mathrm{e}^{\lambda \langle \nu \rangle}(1 - P_0) \mathrm{e}^{-\lambda \langle \nu \rangle} \Psi\|_{\mathcal{H}} \\
&\leq \|\Psi\|_{\mathcal{H}} + \sup_{q \in \mathcal{C}} \|\mathrm{e}^{\lambda \langle \nu \rangle} P_0 \mathrm{e}^{-\lambda \langle \nu \rangle}\|_{\mathcal{L}(\mathcal{H}_{\mathrm{f}}(q))} \|\Psi\|_{\mathcal{H}} \\
&\lesssim \|\Psi\|_{\mathcal{H}},
\end{aligned}
$$

where we used that E_{f} is a constraint energy band by assumption. We now turn to (109). We note that by the Cauchy-Schwarz inequality it suffices to find a $\lambda_0 > 0$ such that for all $\lambda \in [-\lambda_0, \lambda_0]$

$$\langle \Phi | \Phi \rangle_{\mathcal{H}} \lesssim \left| \mathrm{Re} \left\langle \Phi \,\middle|\, \mathrm{e}^{\lambda \langle \nu \rangle}(H_{\mathrm{f}} - E_{\mathrm{f}}) \mathrm{e}^{-\lambda \langle \nu \rangle} \Phi \right\rangle_{\mathcal{H}} \right| \tag{110}$$

To derive (110) we start with the following useful estimate, which is easily obtained by commuting $H_{\mathrm{f}} - E_{\mathrm{f}}$ with $\mathrm{e}^{-\lambda \langle \nu \rangle}$.

$$
\begin{aligned}
\left| \mathrm{Re} \left\langle \Phi \,\middle|\, \mathrm{e}^{\lambda \langle \nu \rangle}(H_{\mathrm{f}} - E_{\mathrm{f}}) \mathrm{e}^{-\lambda \langle \nu \rangle} \Phi \right\rangle \right| &= \left| \langle \Phi |(H_{\mathrm{f}} - E_{\mathrm{f}}) \Phi \rangle - \lambda^2 \langle \Phi |(|\nu|^2 / \langle \nu \rangle^2) \Phi \rangle \right| \\
&\geq \left| \langle \Phi |(H_{\mathrm{f}} - E_{\mathrm{f}}) \Phi \rangle \right| - \lambda^2 \langle \Phi | \Phi \rangle.
\end{aligned}
$$

Since E_{f} is assumed to be a constraint energy band and thus separated by a gap, we have

$$
\begin{aligned}
\left| \langle \Phi |(H_{\mathrm{f}} - E_{\mathrm{f}}) \Phi \rangle \right| &= \left| \left\langle (1 - P_0) \Phi \,\middle|\, (H_{\mathrm{f}} - E_{\mathrm{f}})(1 - P_0) \Phi \right\rangle \right| \\
&\geq c_{\mathrm{gap}} \left\langle (1 - P_0) \Phi \,\middle|\, (1 - P_0) \Phi \right\rangle \\
&= c_{\mathrm{gap}} \left(\langle \Phi | \Phi \rangle - \langle \Phi | P_0 \Phi \rangle \right).
\end{aligned}
$$

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 $\lambda \in [-\lambda_0, \lambda_0]$. Since E_{f} is a constraint energy band by assumption, we know that there are $\Lambda_0 > 0$ and $C < \infty$ independent of $q \in \mathcal{C}$ such that $\|\mathrm{e}^{\Lambda_0 \langle \nu \rangle} P_0(q) \mathrm{e}^{\Lambda_0 \langle \nu \rangle}\|_{\mathcal{H}_{\mathrm{f}}(q)} \leq C$. Hence,

$$
\begin{aligned}
1 = \mathrm{tr}_{\mathcal{H}_{\mathrm{f}}(q)}\left(P_0^2(q)\right) &= \mathrm{tr}_{\mathcal{H}_{\mathrm{f}}(q)}\left(\mathrm{e}^{\Lambda_0 \langle \nu \rangle} P_0(q) \mathrm{e}^{\Lambda_0 \langle \nu \rangle} \mathrm{e}^{-\Lambda_0 \langle \nu \rangle} P_0(q) \mathrm{e}^{-\Lambda_0 \langle \nu \rangle}\right) \\
&\leq \|\mathrm{e}^{\Lambda_0 \langle \nu \rangle} P_0(q) \mathrm{e}^{\Lambda_0 \langle \nu \rangle}\|_{\mathcal{H}_{\mathrm{f}}(q)} \mathrm{tr}_{\mathcal{H}_{\mathrm{f}}(q)}\left(\mathrm{e}^{-\Lambda_0 \langle \nu \rangle} P_0 \mathrm{e}^{-\Lambda_0 \langle \nu \rangle}\right) \\
&\leq C \, \mathrm{tr}_{\mathcal{H}_{\mathrm{f}}(q)}\left(\mathrm{e}^{-\Lambda_0 \langle \nu \rangle} P_0 \mathrm{e}^{-\Lambda_0 \langle \nu \rangle}\right).
\end{aligned}
$$

So we have that for any λ with $\lambda \in [-\Lambda_0, \Lambda_0]$

$$\inf_q \operatorname{tr}_{\mathcal{H}_{\mathrm{f}}(q)}\big(\mathrm{e}^{-\lambda\langle\nu\rangle} P_0(q) \mathrm{e}^{-\lambda\langle\nu\rangle}\big) \ \geq\ \inf_q \operatorname{tr}_{\mathcal{H}_{\mathrm{f}}(q)}\big(\mathrm{e}^{-\Lambda_0\langle\nu\rangle} P_0(q) \mathrm{e}^{-\Lambda_0\langle\nu\rangle}\big) \ \geq\ C^{-1}.$$

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

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

which finishes the proof of (110).

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

$$0 \ = \ (H_{\mathrm{f}} - E_{\mathrm{f}})P_0 \ = \ -\Delta_{\mathrm{v}} P_0 + V_0 P_0 - E_{\mathrm{f}} P_0. \tag{111}$$

Let $\tau_1, \ldots \tau_m \in \Gamma_{\mathrm{b}}(T\mathcal{C})$ be arbitrary. To show that the derivatives of P_0 decay exponentially, we consider equations obtained by commutating the operator identity (111) with $\nabla^{\mathrm{h}}_{\tau_1, \ldots, \tau_m}$. Since Δ_{v} commutes with ∇^{h} by Lemma 8, this yields the following hierachy of equations:

$$
\begin{aligned}
(H_{\mathrm{f}} - E_{\mathrm{f}})(\nabla^{\mathrm{h}}_{\tau_1} P_0) &= (\nabla_{\tau_1} E_{\mathrm{f}} - \nabla^{\mathrm{h}}_{\tau_1} V_0)P_0, \\
(H_{\mathrm{f}} - E_{\mathrm{f}})(\nabla^{\mathrm{h}}_{\tau_1, \tau_2} P_0) &= (\nabla_{\tau_1, \tau_2} E_{\mathrm{f}} - \nabla^{\mathrm{h}}_{\tau_1, \tau_2} V_0)P_0 + (\nabla_{\tau_2} E_{\mathrm{f}} - \nabla^{\mathrm{h}}_{\tau_2} V_0)(\nabla^{\mathrm{h}}_{\tau_1} P_0) \\
&\quad + (\nabla_{\tau_1} E_{\mathrm{f}} - \nabla^{\mathrm{h}}_{\tau_1} V_0)(\nabla^{\mathrm{h}}_{\tau_2} P_0),
\end{aligned}
$$

and analogous equations for higher and mixed derivatives. Applying the reduced resolvent $R_{H_{\mathrm{f}}}(E_{\mathrm{f}})$ to both sides of the first equation we obtain that

$$(1 - P_0)(\nabla^{\mathrm{h}}_{\tau_1} P_0) \ = \ R_{H_{\mathrm{f}}}(E_{\mathrm{f}})(\nabla^{\mathrm{h}}_{\tau_1} E_{\mathrm{f}} - \nabla^{\mathrm{h}}_{\tau_1} V_0)P_0.$$

From $\big\| \mathrm{e}^{\lambda_0\langle\nu\rangle} P_0 \mathrm{e}^{\lambda_0\langle\nu\rangle} \big\|_{\mathcal{L}(\mathcal{H})} \lesssim 1$ we conclude that

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

because the derivatives of V_0 and E_{f} are globally bounded and application of $R_{H_{\mathrm{f}}}(E_{\mathrm{f}})$ preserves exponential decay as we have shown above. Inductively, we obtain that

$$\big\| \mathrm{e}^{\lambda_0\langle\nu\rangle}(1 - P_0)\big(\nabla^{\mathrm{v}}_{\nu_1, \ldots, \nu_l} \nabla^{\mathrm{h}}_{\tau_1, \ldots, \tau_m} P_0\big) \mathrm{e}^{\lambda_0\langle\nu\rangle} \big\|_{\mathcal{L}(\mathcal{H})} \ \lesssim \ 1.$$

The same arguments yield $\left\| e^{\lambda_0\langle\nu\rangle}\big(\nabla^v_{\nu_1,\dots,\nu_l}\nabla^h_{\tau_1,\dots,\tau_m}P_0\big)(1-P_0)e^{\lambda_0\langle\nu\rangle}\right\|_{\mathcal{L}(\mathcal{H})}\lesssim 1$ when we start with $0=P_0(H_f-E_f)$. The assumption $\left\| e^{\lambda_0\langle\nu\rangle}P_0 e^{\lambda_0\langle\nu\rangle}\right\|_{\mathcal{L}(\mathcal{H})}\lesssim 1$ immediately implies $\left\| e^{\lambda_0\langle\nu\rangle}P_0\big(\nabla^v_{\nu_1,\dots,\nu_l}\nabla^h_{\tau_1,\dots,\tau_m}P_0\big)P_0 e^{\lambda_0\langle\nu\rangle}\right\|_{\mathcal{L}(\mathcal{H})}\lesssim 1$. These three statements together result in

$$\left\| e^{\lambda_0\langle\nu\rangle}\big(\nabla^v_{\nu_1,\dots,\nu_l}\nabla^h_{\tau_1,\dots,\tau_m}\big)e^{\lambda_0\langle\nu\rangle}\right\|_{\mathcal{L}(\mathcal{H})}\lesssim 1.$$

We now turn to ii). So we assume that $\varphi_f \in C_b^m(\mathcal{C},\mathcal{H}_f(q))$ for some $m\in\mathbb{N}_0$. By definition φ_f satisfies

$$0 = (H_f-E_f)\varphi_f = -\Delta_v\varphi_f + V_0\varphi_f - E_f\varphi_f. \tag{112}$$

for all $q\in\mathcal{C}$. Because of $V_0\in C_b^\infty(\mathcal{C},C_b^\infty(N_q\mathcal{C}))$ and $E_f\in C_b^\infty(\mathcal{C})$ this is an elliptic equation with coefficients in $C_b^0(\mathcal{C},C_b^\infty(N_q\mathcal{C}))$ on each fibre. Therefore $\varphi_f \in C_b^0(\mathcal{C},C_b^\infty(N_q\mathcal{C}))$ follows from $\varphi_f \in C_b^0(\mathcal{C},\mathcal{H}_f(q))$ and standard elliptic theory immediately. Due to $\varphi_f\in C_b^m(\mathcal{C},\mathcal{H}_f(q))$ we may take horizontal derivatives of (112). Using that $[\Delta_v,\nabla^h_\tau]$ for all τ by Lemma 8 ii), we end up with the following equations

$$\begin{aligned}(H_f-E_f)\nabla^h_{\tau_1}\varphi_f &= (\nabla_{\tau_1}E_f - \nabla^h_\tau V_0)\varphi_f, \tag{113}\\ (H_f-E_f)\nabla^h_{\tau_1,\tau_2}\varphi_f &= (\nabla_{\tau_1,\tau_2}E_f-\nabla^h_{\tau_1,\tau_2}V_0)\varphi_f + (\nabla_{\tau_1}E_f-\nabla^h_{\tau_1}V_0)(\nabla^h_{\tau_2}\varphi_f)\\ &\quad + (\nabla_{\tau_2}E_f-\nabla^h_{\tau_2}V_0)(\nabla^h_{\tau_1}\varphi_f),\end{aligned}$$

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 $\varphi_f\in C_b^m(\mathcal{C},C_b^\infty(N_q\mathcal{C}))$. So we may take also vertical derivatives of the above hierachy:

$$\begin{aligned}(H_f-E_f)\nabla^v_{\nu_1}\varphi_f &= -(\nabla^v_{\nu_1}V_0)\,\varphi_f, \tag{114}\\ (H_f-E_f)\nabla^v_{\nu_1}\nabla^h_{\tau_1}\varphi_f &= -(\nabla^v_{\nu_1}\nabla^h_{\tau_1}V_0)\varphi_f - (\nabla^v_{\nu_1}V_0)(\nabla^h_{\tau_1}\varphi_f)\\ &\quad + (\nabla_{\tau_1}E_f-\nabla^h_{\tau_1}V_0)\nabla^v_{\nu_1}\varphi_f)\end{aligned}$$

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

$$\left\| e^{\Lambda_0\langle\nu\rangle}\varphi_f\,\langle e^{\Lambda_0\langle\nu\rangle}\varphi_f|\psi\rangle_{\mathcal{H}_f(q)}\right\|_{\mathcal{H}_f(q)} = \left\| e^{\Lambda_0\langle\nu\rangle}P_0 e^{\Lambda_0\langle\nu\rangle}\psi\right\|_{\mathcal{H}_f(q)} \lesssim \|\psi\|_{\mathcal{H}_f(q)}$$

with a constant independent of q. Choosing $\psi = e^{-\Lambda_0\langle\nu\rangle}\varphi_f$ and taking the supremum over $q\in\mathcal{C}$ we obtain the desired exponential decay of φ_f. Because of $V_0\in C_b^\infty(\mathcal{C},C_b^\infty(N_q\mathcal{C}))$ and $E_f\in C_b^\infty(\mathcal{C})$ also the right-hand sides of (113) and (114) decay exponentially. By i) an application of $R_{H_f}(E_f)$ preserves exponential decay. So we may conclude that the φ_f-orthogonal parts of $\nabla^h_{\tau_1}\varphi_f$

and $\nabla^{\mathrm{v}}_{\nu_1} \varphi_{\mathrm{f}}$ decay exponentially. Together with the exponential decay of φ_{f} this entails the desired exponential decay of $\nabla^{\mathrm{h}}_{\tau_1} \varphi_{\mathrm{f}}$ and $\nabla^{\mathrm{v}}_{\nu_1} \varphi_{\mathrm{f}}$. This argument can now easily be iterated for the higher derivatives.

Finally, we turn to iii). We consider a normalized trivializing section φ_{f}, in particular $\sup_{q \in \mathcal{C}} \|\varphi_{\mathrm{f}}\|_{\mathcal{H}_{\mathrm{f}}}$ is globally bounded. f By assumption φ_{f} is smooth as a section of $P_0 \mathcal{H}$. In order to see that it is also smooth in $(1 - P_0)\mathcal{H}$, one applies $R_{H_{\mathrm{f}}}(E_{\mathrm{f}})$ to the equations (113), 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.

We recall that the eigenfunction $\varphi_{\mathrm{f}}(q)$ can be chosen real-valued for any $q \in \mathcal{C}$. 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_{f}. We choose a covering of $\mathcal{C}$ by geodesic balls of fixed diameter and take an arbitrary one of them called Ω. We choose geodesic coordinates $(x^i)_{i=1,\ldots,d}$ and bundle coordinates $(n^\alpha)_{\alpha=1,\ldots,k}$ with respect to an orthonormal trivializing frame $(\nu_\alpha)_\alpha$ over Ω as in Remark 5. Since φ_{f} is the only normalized element of the real $P_0 \mathcal{H}$, we have that

$$\varphi_{\mathrm{f}}(q) = \frac{P_0(x)\varphi_{\mathrm{f}}(x_0)}{\|P_0(x)\varphi_{\mathrm{f}}(x_0)\|} \tag{115}$$

for any fixed $x_0 \in \Omega$ and x close to it. In view of the coordinate expression $\nabla^{\mathrm{h}}_{\partial_{x^i}} = \partial_{x^i} - \Gamma^\alpha_{i\beta} n^\beta \partial_{n^\alpha}$, we can split up $\nabla^{\mathrm{h}}_{\partial_{x^i}} \varphi_{\mathrm{f}}$ into terms depending on $\nabla^{\mathrm{h}}_{\partial_{x^i}} P_0$, which are bounded due to i), and $-\Gamma^\alpha_{i\beta} n^\beta \partial_{n^\alpha} \varphi_{\mathrm{f}}(x_0)$. We already know that $\varphi_{\mathrm{f}} \in C^0_{\mathrm{b}}\big(\mathcal{C}, \mathcal{H}_{\mathrm{f}}(q)\big)$. By ii) this implies $\varphi_{\mathrm{f}} \in C^0_{\mathrm{b}}\big(\mathcal{C}, C^\infty_{\mathrm{b}}(N_q\mathcal{C})\big)$ with $\sup_q \|\mathrm{e}^{\lambda_0 \langle \nu \rangle} \varphi_{\mathrm{f}}\| \lesssim 1$. Recalling that $\langle \nu \rangle = \sqrt{1 + \delta_{\alpha\beta} n^\alpha n^\beta}$ we have that $-\Gamma^\alpha_{i\beta} n^\beta \partial_{n^\alpha} \varphi_{\mathrm{f}}(x_0)$ is bounded. Noticing that all the bounds are independent of Ω due to (13) (as was explained in Remark 5) we obtain that $\varphi_{\mathrm{f}} \in C^1_{\mathrm{b}}\big(\mathcal{C}, \mathcal{H}_{\mathrm{f}}(q)\big)$. Now we can inductively make use of (115) and ii) to obtain $\varphi_{\mathrm{f}} \in C^\infty_{\mathrm{b}}\big(\mathcal{C}, \mathcal{H}_{\mathrm{f}}(q)\big)$.

If $E_{\mathrm{f}} = \inf \sigma(H_{\mathrm{f}}(q))$ for all $q \in \mathcal{C}$, again the real eigenspace bundle is already trivializable. To see this we note that the groundstate of a Schrödinger operator with a bounded potential can always be chosen strictly positive (see [37]), 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 $\mathcal{C}$ that the derivatives are globally bounded. $\qquad\square$

PROOF OF LEMMA 12:
Let the assumption (96) be true for $l \in \mathbb{N}_0$ and $m \in \mathbb{N}$. The proof for $-l \in \mathbb{N}$ is very similar. We fix $z_1, \ldots, z_m \in (\mathbb{C} \setminus \mathbb{R}) \cap (\operatorname{supp} \chi \times [-1, 1])$ and claim

that there is a $c > 0$ independent of the z_i such that

$$\left\| \prod_{i=1}^{m}(H - z_i)\, \langle \lambda\nu \rangle^l \prod_{j=1}^{m} R_H(z_j)\, \langle \lambda\nu \rangle^{-l} \right\|_{\mathcal{L}(\mathcal{H})} \leq 2 \qquad (116)$$

for $\lambda := \min\left\{ 1, C_1^{-1}\, \frac{c\,\prod_{i=1}^{m}|\mathrm{Im}z_i|}{1+\prod_{j=1}^{m}(|z_j|+|\mathrm{Im}z_j|)} \right\} > 0$.

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

$$
\begin{aligned}
\|\Psi\| &= \left\| \langle \lambda\nu \rangle^l \prod_{j=1}^{m}(H - z_i)\, \langle \lambda\nu \rangle^{-l} \prod_{i=1}^{m} R_H(z_j)\, \Phi \right\| \\[2mm]
&\geq \|\Phi\| - \left\| \langle \lambda\nu \rangle^l \left[\prod_{j=1}^{m}(H - z_i), \langle \lambda\nu \rangle^{-l} \right] \prod_{i=1}^{m} R_H(z_j)\, \Phi \right\|
\end{aligned}
$$

Using the assumption (96) and that $|z_i| \leq 1$ for all i we have that there is a $C < \infty$ independent of λ and the z_i's with

$$
\begin{aligned}
\|\Psi\| &\geq \|\Phi\| - C\,C_1\lambda \left(\left\| H^m \prod_{j=1}^{m} R_H(z_j)\, \Phi \right\| + \left\| \prod_{j=1}^{m} R_H(z_j)\, \Phi \right\| \right) \\[2mm]
&= \|\Phi\| - C\,C_1\lambda \left\| \prod_{j=1}^{m} H\,R_{H_\varepsilon}(z_j)\, \Phi \right\| - C\,C_1\lambda \left\| \prod_{j=1}^{m} R_H(z_j)\, \Phi \right\| \\[2mm]
&\geq \|\Phi\| - C\,C_1\lambda \prod_{j=1}^{m}\left(1 + \frac{|z_j|}{|\mathrm{Im}z_j|} \right)\|\Phi\| - C\,C_1\lambda \prod_{j=1}^{m} |\mathrm{Im}z_j|^{-1}\,\|\Phi\| \\[2mm]
&\geq \|\Phi\| - C\,C_1\lambda\, \frac{1 + \prod_{j=1}^{m}(|z_j| + |\mathrm{Im}z_j|)}{\prod_{i=1}^{m} |\mathrm{Im}z_i|}\,\|\Phi\| \\[2mm]
&\geq \|\Phi\|/2
\end{aligned}
$$

for $\lambda \leq C_1^{-1}\, \frac{(2C)^{-1}\,\prod_{i=1}^{m}|\mathrm{Im}z_i|}{1+\prod_{j=1}^{m}(|z_j|+|\mathrm{Im}z_j|)}$. This yields (116).

Now we make use of the Helffer-Sjöstrand formula. We recall from the proof of Lemma 7 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. Here by dz we mean again the usual volume measure on $\mathbb{C}$. By assumption χ is non-negative. So by the spectral theorem we have $\chi(H) = \prod_{i=1}^{m} \chi^{1/m}(H)$. We choose an almost

analytic extension of $\chi^{1/m}$ such that $K := \mathrm{supp}\,\widetilde{\chi^{1/m}} \subset \mathrm{supp}\,\chi \times [-1,1]$ (in particular the volume of K is finite) and

$$|\widetilde{\partial_{\bar{z}}\chi^{1/m}}(z)| \;=\; \mathcal{O}(|\mathrm{Im}z|^{l+1}). \tag{117}$$

Then by the Helffer-Sjöstrand formula

$$\chi(H) \;=\; \frac{1}{\pi^m} \int_{\mathbb{C}^m} \prod_{i=1}^m \widetilde{\partial_{\bar{z}}\chi^{1/m}}(z_i) \prod_{i=1}^m R_H(z_i)\, dz_1 \ldots dz_m.$$

We will now combine (116) and (117) to obtain the claimed estimate. In the following, we use $\lesssim$ for 'bounded by a constant independent of H'.

$$\left| \langle\nu\rangle^l \chi(H) \langle\nu\rangle^{-l} \Psi \right|$$
$$= \left| \frac{1}{\pi^m} \int_{\mathbb{C}^m} \prod_{i=1}^m \widetilde{\partial_{\bar{z}}\chi^{1/m}}(z_i)\langle\nu\rangle^l\langle\lambda\nu\rangle^{-l}\, \langle\lambda\nu\rangle^l \prod_{i=1}^m R_H(z_i)\langle\nu\rangle^{-l}\Psi\, dz_1 \ldots dz_m \right|$$
$$\overset{(117)}{\lesssim} C_1^l \int_{K^m} \prod_{i=1}^m |\mathrm{Im}z_i| \left| \langle\lambda\nu\rangle^l \prod_{i=1}^m R_H(z_i)\langle\nu\rangle^{-l}\,\Psi \right| dz_1 \ldots dz_m$$

where we used that $\langle\nu\rangle^l\langle\lambda\nu\rangle^{-l} \le \lambda^{-l} \sim C_1^l \prod_{i=1}^m |\mathrm{Im}\,z_i|^{-l}$ for small $|\mathrm{Im}\,z_i|$. So

$$\left\| \langle\nu\rangle^l \chi(H) \langle\nu\rangle^{-l} \Psi \right\|_{\mathcal{D}(H^m)}$$
$$\lesssim C_1^l \left\| \int_{K^m} \prod_{i=1}^m |\mathrm{Im}z_i| \left| \langle\lambda\nu\rangle^l \prod_{i=1}^m R_H(z_i)\, \langle\nu\rangle^{-l}\,\Psi \right| dz_1 \ldots dz_m \right\|_{\mathcal{D}(H^m)}$$
$$= C_1^l \left\| \int_{K^m} \prod_{i=1}^m |\mathrm{Im}z_i| \left| \prod_{i=1}^m R_H(z_i) \prod_{i=1}^m (H - z_i)\, \langle\lambda\nu\rangle^l \right. \right.$$
$$\left. \left. \times \prod_{i=1}^m R_H(z_i)\langle\lambda\nu\rangle^{-l}\, \langle\lambda\nu\rangle^l\, \langle\nu\rangle^{-l}\,\Psi \right| dz_1 \ldots dz_m \right\|_{\mathcal{D}(H^m)}$$
$$\le C_1^l \int_{K^m} \prod_{i=1}^m |\mathrm{Im}z_i| \prod_{i=1}^m \|R_H(z_i)\|_{\mathcal{L}(\mathcal{D}(H^{m-i}),\mathcal{D}(H^{m-i+1}))} \, \|\langle\lambda\nu\rangle^l\, \langle\nu\rangle^{-l}\,\Psi\|_{\mathcal{H}}$$
$$\times \left\| \prod_{i=1}^m (H_\varepsilon - z_i)\, \langle\lambda\nu\rangle^l \prod_{i=1}^m R_{H_\varepsilon}(z_i)\langle\lambda\nu\rangle^{-l} \right\|_{\mathcal{L}(\mathcal{H})} dz_1 \ldots dz_m$$
$$\overset{(116)}{\lesssim} C_1^l \,\|\Psi\|_{\mathcal{H}},$$

because of the resolvent estimate (70) and $\langle\lambda\nu\rangle^l\langle\nu\rangle^{-l} \le 1$ for $\lambda \le 1$. Hence, $\|\langle\nu\rangle^l\chi(H)\,\langle\nu\rangle^{-l}\|_{\mathcal{L}(\mathcal{H},\mathcal{D}(H_\varepsilon^m))}$ is bounded by C_1^l times a constant independent of H. $\qquad\square$

Appendix

Manifolds of bounded geometry

Here we explain shortly the notion of bounded geometry, which provides the natural framework for this work. More on the subject can be found in [40].

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.*

$$\forall\, m \in \mathbb{N}\ \ \exists\, C_m < \infty: \quad g(\nabla^m \mathcal{R}, \nabla^m \mathcal{R})\ \leq\ C_m. \tag{118}$$

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. An open subset $U \subset \mathcal{M}$ equipped with the induced metric $g|_U$ is called a subset of bounded geometry, if $r_{\mathcal{M}} > 0$ and (118) is satisfied on U.

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 up to any order. Finally, we note that the closure of a subset of bounded geometry is obviously metrically complete.

The geometry of submanifolds

We recall here some standard concepts from Riemannian geometry. For further information see e.g. [23].
First we give the definitions of the inner curvature tensors we use because they vary in the literature. We note that they contain statements about tensoriality 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 $(\mathcal{A}, \overline{g})$ be a Riemannian manifold with Levi-Civita connection $\overline{\nabla}$. Let $\tau_1, \tau_2, \tau_3, \tau_4 \in \Gamma(T\mathcal{A})$.*
i) The curvature mapping $\overline{\mathrm{R}} : \Gamma(T\mathcal{A}) \times \Gamma(T\mathcal{A}) \to \mathcal{T}_1^1(\mathcal{A})$ *is given by*

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

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

$$\overline{\mathcal{R}}(\tau_1, \tau_2, \tau_3, \tau_4)\ :=\ \overline{g}\big(\tau_1, \overline{\mathrm{R}}(\tau_3, \tau_4)\, \tau_2\big).$$

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

$$\overline{\mathrm{Ric}}(\tau_1, \tau_2) \ := \ \mathrm{tr}_{\mathcal{A}}\,\overline{\mathrm{R}}(\,.\,, \tau_1)\tau_2.$$

iv) The scalar curvature $\overline{\kappa} : \mathcal{A} \to \mathbb{R}$ *is given by*

$$\overline{\kappa} \ := \ \mathrm{tr}_{\mathcal{A}}\,\overline{\mathrm{Ric}}.$$

Here $\mathrm{tr}_{\mathcal{A}}\,t$ *means contracting the tensor* t *at any point* $q \in \mathcal{A}$ *by an arbitrary orthonormal basis of* $T_q\mathcal{A}$.

Remark 6 *The dependence on vector fields of* $\overline{\mathrm{R}}$, $\overline{\mathcal{R}}$, *and* $\overline{\mathrm{Ric}}$ *can be lifted to the cotangent bundle* $T\mathcal{C}^*$ *via the metric* $\overline{g}$. *The resulting objects are denoted by the same letters throughout this work. 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* $T\mathcal{C}$ *and* $N\mathcal{C}$ *the tangent and the normal bundle of* $\mathcal{C}$. *Let* $\tau_1, \tau_2, \tau_3 \in \Gamma(T\mathcal{C})$.
i) We define ∇ *to be the* induced connection *on* $\mathcal{C}$ *given via*

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

where τ_1, τ_2 *are canonically lifted to* $T\mathcal{A} = T\mathcal{C} \times N\mathcal{C}$ *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) R, Ric, *and* κ *are defined analogously with* $\overline{\mathrm{R}}$, $\overline{\mathrm{Ric}}$ *and* $\overline{\kappa}$ *from the preceding definition.*

We note that ∇ coincides with the Levi-Civita connection associated to the induced metric g. 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 $\mathcal{W} : \Gamma(N\mathcal{C}) \to \mathcal{T}_1^1(\mathcal{C})$ *is given by*

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

ii) The second fundamental form $\mathrm{II}(\,.\,) : \Gamma(N\mathcal{C}) \to \mathcal{T}_2^0(\mathcal{C})$ *is defined by*

$$\mathrm{II}(\nu)\big(\tau_1, \tau_2\big) \ := \ \overline{g}\big(\overline{\nabla}_{\tau_1}\tau_2, \nu\big).$$

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

$$\overline{g}(\eta, \nu) \ = \ \operatorname{tr}_{\mathcal{C}}\mathcal{W}(\nu) \qquad \forall \ \nu \in \Gamma(N\mathcal{C}).$$

iv) We define the normal connection $\nabla^{\perp}$ *to be the bundle connection on the normal bundle given via*

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

where ν and τ are canonically lifted to $T\mathcal{A} = T\mathcal{C} \times N\mathcal{C}$.
v) $\mathrm{R}^{\perp} : \Gamma(T\mathcal{C}) \times \Gamma(T\mathcal{C}) \times \Gamma(N\mathcal{C}) \rightarrow \Gamma(N\mathcal{C})$ denotes the normal curvature mapping *defined by*

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

Remark 7 *i) The usual relations and symmetry properties for $\mathcal{W}$ and II also hold for codimension greater than one:*

$$\mathrm{II}(\nu)(\tau_1, \tau_2) = g\big(\tau_1, \mathcal{W}(\nu)\, \tau_2\big) = g\big(\tau_2, \mathcal{W}(\nu)\, \tau_1\big) = \mathrm{II}(\nu)(\tau_2, \tau_1).$$

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

$$\nabla^{\perp}_{\tau}\nu \ = \ \overline{\nabla}_{\tau}\nu \ + \ \mathcal{W}(\nu)\tau.$$

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

References

[1] D. E. Blair, *Riemannian Geometry of Contact and Symplectic Manifolds*, Progress in Mathematics **203**, Birkhäuser (2002).

[2] F. Bornemann, *Homogenization in time of singularly perturbed mechanical systems*, Lecture Notes in Mathematics **1687**, Springer (1998).

[3] R. Bott, L. W. Tu, *Differential Forms in Algebraic Topology*, Graduate Texts in Mathematics **82**, Springer (1982).

[4] J.-L. Brylinski, *Loop Spaces, Characteristc Classes and Geometric Quantization*, Progress in Mathematics **107**, Birkhäuser (1993).

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

[6] J. Brüning, S. Yu. Dobrokhotov, V. Nekrasov, T. Ya. Tudorovskiy, *Quantum dynamics in a thin film. I. Propagation of localized perturbations*, Russ. J. Math. Phys. **15**, 1–16 (2008).

[7] M. P. do Carmo, *Differential Geometry of Curves and Surfaces*, Prentice-Hall (1976).

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

[9] E. B. Davies, *Spectral Theory and Differential Operators*, Cambridge studies in advanced mathematics **42**, Cambridge University Press (1995).

[10] G. F. Dell'Antonio, L. Tenuta, *Semiclassical analysis of constrained quantum systems*, J. Phys. A **37**, 5605–5624 (2004).

[11] P. A. M. Dirac, *Lectures on Quantum Mechanics*, Yeshiva Press (1964).

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

[13] N. Dunford, J. T. Schwartz, *Linear operators part I: general theory*, Pure and applied mathematics **7**, Interscience publishers, inc. (1957).

[14] L. Friedlander, M. Solomyak, *On the spectrum of the Dirichlet Laplacian in a narrow strip, II*, arXiv:0710.1886v1 [math.SP].

[15] R. Froese, I. Herbst, *Realizing Holonomic Constraints in Classical and Quantum Mechanics*, Commun. Math. Phys. **220**, 489–535 (2001).

[16] D. Grieser, *Thin tubes in mathematical physics, global analysis and spectral geometry*, in Analysis on Graphs and its Applications, Proc. Sympos. Pure Math. 77, Amer. Math. Soc., 565–593 (2008).

[17] E. Hairer, Ch. Lubich, G. Wanner, *Geometric numerical integration. Structure-preserving algorithms for ordinary differential equations*, Second edition, Springer (2006).

[18] B. Helffer, J. Sjöstrand, *Multiple wells in the semi-classical limit I*, Commun. Part. Diff. Eq. **9**, 337–408 (1984).

[19] P. D. Hislop, *Exponential decay of two-body eigenfunctions: A review*, Elec. J. Diff. Eq. **04**, 265–288 (2000).

[20] M. Jääskeläinen, S. Stenholm, *Localization in splitting of matter waves*, Phys. Rev. A **68**, 033607 (2003).

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

[22] D. Krejčiřík, *Twisting versus bending in quantum wave guides*, in Analysis on Graphs and its Applications, Proc. Sympos. Pure Math. 77, Amer. Math. Soc., 617–636 (2008).

[23] S. Lang, *Fundamentals of Differential Geometry*, Graduate Texts in Mathematics **191**, Springer, (1999).

[24] M.-C. Liu, *Affine maps of tangent bundles with Sasaki metric*, Tensor (N.S.) **28**, 34 –42 (1974).

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

[26] P. Maraner, *Monopole Gauge Fields and Quantum potentials Induced by the Geometry in Simple Dynamical Systems*, Annals of Physics **246**, 325–346 (1996).

[27] R. A. Marcus, *On the Analytical Mechanics of Chemical Reactions. Quantum Mechanics of Linear Collisions*, J. Chem. Phys. **45**, 4493–4499 (1966).

[28] A. Martinez, V. Sordoni, *On the Time-Dependent Born-Oppenheimer Approximation with Smooth Potential*, Comptes Rendus Acad. Sci. Paris **337**, 185 –188 (2002).

[29] A. Martinez, V. Sordoni, *Twisted pseudodifferential calculus and application to the quantum evolution of molecules*, Mem. Amer. Math. Soc. **200**, no. 936 (2009).

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

[31] G. Nenciu, *Linear Adiabatic Theory, Exponential Estimates*, Comm. Math. Phys. **152**, 479–496 (1993).

[32] G. Nenciu, V. Sordoni, *Semiclassical limit for multistate Klein-Gordon systems: almost invariant subspaces and scattering theory*, J. Math. Phys. **45**, 3676–3696 (2004).

[33] G. Panati, *Triviality of Bloch and Bloch-Dirac bundles*, Ann. Henri Poincaré **8**, 995-1011 (2007).

[34] G. Panati, H. Spohn, S. Teufel, *The time-dependent Born-Oppenheimer approximation*, Math. Modelling and Num. Anal. **41**, 297–314 (2007).

[35] M. Reed, B. Simon, *Methods of Modern Mathematical Physics I: Functional Analysis*, Academic Press (1978).

[36] M. Reed, B. Simon, *Methods of Modern Mathematical Physics II: Fourier Analysis, Self-Adjointness*, Academic Press (1978).

[37] M. Reed, B. Simon, *Methods of Modern Mathematical Physics IV: Analysis of Operators*, Academic Press (1978).

[38] H. Rubin, P. Ungar, *Motion under a strong constraining force*, Commun. Pure Appl. Math. **10**, 28–42 (1957).

[39] T. Sakai, *Riemannian Geometry*, Translations of Mathematical Monographs **149**, AMS (1997).

[40] M. A. Shubin, *Spectral theory of elliptic operators on non-compact manifolds*, Asterisque **207**, 35–108 (1992).

[41] V. Sordoni, *Reduction Scheme for Semiclassical Operator–Valued Schrödinger Type Equation and Application to Scattering*, Commun. Part. Diff. Eq. **28**, 1221–1236 (2003).

[42] L. Tenuta, S. Teufel, *Effective dynamics for particles coupled to a quantized scalar field*, Commun. Math. Phys. **280**, 751–805 (2008).

[43] S. Teufel, *Adiabatic Perturbation Theory in Quantum Dynamics*, Lecture Notes in Mathematics **1821**, Springer (2003).

[44] O. Wittich, L^2-*Homogenization of Heat Equations on Tubular Neighborhoods*, arXiv:0810.5047v1 [math.AP].