ABSENCE OF POSITIVE EIGENVALUES FOR HARD-CORE N-BODY SYSTEMS

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Abstract. We show absence of positive eigenvalues for generalized 2-body hard-core Schrödinger operators under the condition of bounded strictly convex obstacles. A scheme for showing absence of positive eigenvalues for generalized N-body hard-core Schrödinger operators, $N \geq 2$, is presented. This scheme involves high energy resolvent estimates, and for $N = 2$ it is implemented by a Mourre commutator type method. A particular example is the Helium atom with the assumption of infinite mass and finite extent nucleus.

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1. Introduction and results

Consider the N-body Schrödinger operator

$$H = \sum_{j=1}^{N} \Big(-\frac{1}{2m_j} \Delta_{x_j} + V_j^{\mathrm{ncl}}(x_j) \Big) + \sum_{1 \leq i < j \leq N} V_{ij}^{\mathrm{elec}}(x_i - x_j) \tag{1.1}$$

for a system of N d-dimensional particles in the exterior of a bounded strictly convex obstacle $\Theta_1 \subset \mathbb{R}^d$ (for $N = 1$ the last term is omitted). Whence H is an operator on the Hilbert space $L^2(\Omega)$; $\Omega = (\Omega_1)^N$, $\Omega_1 = \mathbb{R}^d \setminus \overline{\Theta}_1$. It is defined more precisely by imposing the Dirichlet boundary condition. This operator models a system of N d-dimensional charged particles interacting with a fixed charged nucleus of finite extent, for example a ball (or possibly a somewhat deformed ball). In particular (assuming $0 \in \Theta_1$) we could have Coulomb interactions $V_j^{\mathrm{ncl}}(y) = q_j q^{\mathrm{ncl}}|y|^{-1}$ and $V_{ij}^{\mathrm{elec}}(y) = q_i q_j |y|^{-1}$ in dimension $d \geq 2$. We address the problem of proving absence of positive eigenvalues. While this property is well-known for the one-body problem it is open for $N \geq 2$. We introduce for obstacle problems of this type a general procedure involving high energy resolvent estimates for effective sub-Hamiltonians. We show that this scheme can be implemented for the case $N = 2$. In this case essentially such an effective sub-Hamiltonian is a one-body Hamiltonian for an exterior region. The result is shown in the so-called generalized 2-body hard-core framework.

1.1. **Usual generalized N-body systems.** We will work in a generalized framework. We first review the analogue of this without obstacles, i.e. with "soft potentials". This is given by real finite dimensional vector space $\mathbf{X}$ with an inner product q, i.e. $(\mathbf{X}, q)$ is Euclidean space, and a finite family of subspaces $\{\mathbf{X}_a |\ a \in \mathcal{A}\}$ closed with respect to intersection. We refer to the elements of $\mathcal{A}$ as *cluster decompositions* (not to be motivated here). The orthogonal complement of $\mathbf{X}_a$ in $\mathbf{X}$ is denoted $\mathbf{X}^a$, and correspondingly we decompose $x = x^a \oplus x_a \in \mathbf{X}^a \oplus \mathbf{X}_a$. We order $\mathcal{A}$ by writing $a_1 \subset a_2$ if $\mathbf{X}^{a_1} \subset \mathbf{X}^{a_2}$. It is assumed that there exist $a_{\min}, a_{\max} \in \mathcal{A}$ such that $\mathbf{X}^{a_{\min}} = \{0\}$ and $\mathbf{X}^{a_{\max}} = \mathbf{X}$. Let $\mathcal{B} = \mathcal{A} \setminus \{a_{\min}\}$. The length of a chain of cluster decompositions $a_1 \subsetneq \cdots \subsetneq a_k$ is the number k. Such a chain is said to connect $a = a_1$ and $b = a_k$. The maximal length of all chains connecting a given $a \in \mathcal{A} \setminus \{a_{\max}\}$ and $a_{\max}$ is denoted by $\#a$. We define $\#a_{\max} = 1$ and denoting $\#a_{\min} = N + 1$ we say the family $\{\mathbf{X}^a | a \in \mathcal{A}\}$ is of N-body type. Whence the generalized 2-body framework is characterized by the condition $\mathbf{X}_a \cap \mathbf{X}_b = \{0\}$ for $a, b \neq a_{\min}$, $a \neq b$.

The N-body Schrödinger operator H introduced above (now considered without an obstacle) can be written on the form

$$H = H_0 + V$$

where $2H_0$ is (minus) the Laplace-Beltrami operator on the space

$$\mathbf{X} = (\mathbb{R}^d)^N, \quad q = \sum_{j=1}^{N} m_j |x_j|^2,$$

$V = V(x) = \sum_{b \in \mathcal{B}} V_b(x^b)$ and indeed the relevant family $\{\mathbf{X}^a | a \in \mathcal{A}\}$ of subspaces as discussed above is of N-body type. However this is just one example of a generalized N-body Schrödinger operator. The general construction of such an operator H is similar, and under the following condition it is well-defined with form domain given by the Sobolev space $H^1(\mathbf{X})$, cf. [RS, Theorem X.17].

Condition 1.1. There exists $\varepsilon > 0$ such that for potential V_b, $b \in \mathcal{B}$, there is a splitting $V_b = V_b^{(1)} + V_b^{(2)}$, where

(1) $V_b^{(1)}$ is smooth and

$$\partial_y^\alpha V_b^{(1)}(y) = O\big(|y|^{-\varepsilon - |\alpha|}\big). \tag{1.2}$$

(2) $V_b^{(2)}$ is compactly supported and

$$(-\Delta+1)^{-1/2}V_b^{(2)}(-\Delta+1)^{-1/2} \text{ is compact on } L^2(\mathbb{R}_y^{\dim \mathbf{X}^b}). \tag{1.3}$$

Let $-\Delta^a=(p^a)^2$ and $-\Delta_a=p_a^2$ denote (minus) the Laplacians on $L^2(\mathbf{X}^a)$ and $L^2(\mathbf{X}_a)$, respectively. Here $p^a=\pi^a p$ and $p_a=\pi_a p$ denote the internal (i.e. within clusters) and the inter-cluster components of the momentum operator $p=-\mathrm{i}\nabla$, respectively. For $a\in\mathcal{B}$, denote

$$\begin{aligned} V^a(x^a)&=\sum_{b\subset a}V_b(x^b),\\ H^a&=-\tfrac12\Delta^a+V^a(x^a),\\ H_a&=H^a-\tfrac12\Delta_a,\\ I_a(x)&=\sum_{b\not\subset a}V_b(x^b). \end{aligned}$$

We define $H^{a_{\min}}=0$ on $L^2(\mathbf{X}^{a_{\min}}):=\mathbb{C}$. The operator H^a is the sub-Hamiltonian associated with the cluster decomposition a and I_a is the sum of all inter-cluster interactions. The detailed expression of H^a depends on the choice of coordinates on $\mathbf{X}^a$.

In a natural way we have sub-Hamiltonians H^a and "inter-cluster" Hamiltonians $H_a=H^a\otimes I+I\otimes\frac12p_a^2$. Given a family $\{\mathbf{X}^a|a\in\mathcal{A}\}$ of N-body type and imposing Condition 1.1 the generalized N-body Hamiltonian is $H=H^{a_{\max}}$.

Let

$$\mathcal{T}=\cup_{a\in\mathcal{A},\#a\geq2}\,\sigma_{\mathrm{pp}}(H^a)$$

be the set of thresholds of H. The HVZ theorem [RS, Theorem XIII.17] gives the bottom of the essential spectrum of H by the formula

$$\inf\sigma_{\mathrm{ess}}(H)=\min_{a\in\mathcal{A}\setminus\{a_{\max}\}}\inf\sigma(H^a)=\min_{a\in\mathcal{A},\#a=2}\inf\sigma(H^a). \tag{1.4}$$

It is also well-known that under rather general conditions H does not have positive eigenvalues and the negative eigenvalues can at most accumulate at the thresholds from below, see [FH] and [Pe].

1.1.1. *Graf vector field.* We give a brief review of the construction of a family of conjugate operators for N-body Hamiltoninans originating from [Sk1]. A slightly different proof appears in [Sk2]. This construction is based on the vector field invented by Graf [Gra] which is a vector field satisfying the following properties, cf. [Sk2, Lemma 4.3]. We use throughout the paper the notation $\langle x\rangle=\sqrt{x^2+1}$ and $\mathbb{N}_0=\mathbb{N}\cup\{0\}$.

Lemma 1.2. *There exist on $\mathbf{X}$ a smooth vector field ω with symmetric derivative ω_* and a partition of unity $\{\tilde q_a\}$ indexed by $a\in\mathcal{A}$ and consisting of smooth functions, $0\leq\tilde q_a\leq1$, such that for some positive constants r_1 and r_2*

(1) $\omega_*(x)\geq\sum_a\pi_a\tilde q_a$.
(2) $\omega^a(x)=0$ *if* $|x^a|<r_1$.
(3) $|x^b|>r_1$ *on* $\operatorname{supp}(\tilde q_a)$ *if* $b\not\subset a$.
(4) $|x^a|<r_2$ *on* $\operatorname{supp}(\tilde q_a)$.
(5) *For all* $\alpha\in\mathbb{N}_0^{\dim\mathbf{X}}$ *and* $k\in\mathbb{N}_0$ *there exist* $C\in\mathbb{R}$:

$$|\partial_x^\alpha\tilde q_a|+|\partial_x^\alpha(x\cdot\nabla)^k\big(\omega(x)-x\big)|\leq C. \tag{1.5}$$

Now, proceeding as in [Sk2], we introduce the rescaled vector field $\omega_R(x) := R\omega(\frac{x}{R})$ and the corresponding operator

$$A = A_R = \omega_R(x) \cdot p + p \cdot \omega_R(x);\ R > 1.$$

We also introduce a function $d : \mathbb{R} \to \mathbb{R}$ by

$$d(E) = \begin{cases} \inf_{\tau \in \mathcal{T}(E)}(E - \tau),\ \mathcal{T}(E) := \mathcal{T} \cap]-\infty, E] \neq \emptyset, \\ 1,\ \mathcal{T}(E) = \emptyset. \end{cases} \tag{1.6}$$

These devices enter into the following Mourre estimate. We remark that all inputs needed for the proof are stated in Lemma 1.2 and that although [Sk2, Corollary 4.5] is stated for relatively operator compact potentials the proof of [Sk2] generalizes to include the class of relatively form compact potentials of Condition 1.1. For a different proof (valid in the context of hard-core interactions) we refer to [Gri] (see also [BGS]).

Lemma 1.3. *For all $E \in \mathbb{R}$ and $\epsilon > 0$ the exists $R_0 > 1$ such that for all $R \geq R_0$ there is a neighbourhood $\mathcal{V}$ of E and a compact operator K on $L^2(\mathbf{X})$ such that*

$$f(H)^* \mathrm{i}[H, A_R] f(H) \geq f(H)^* \{4d(E) - \epsilon - K\} f(H) \text{ for all } f \in C_c^\infty(\mathcal{V}). \tag{1.7}$$

Here the commutator is given by (1.13) stated below. The possibly existing local singularities of the potential do not enter (for R large) due to Lemma 1.2 (2). This feature motivates application to hard-core models, see Subsection 1.2.

Two of the consequences of a Mourre estimate like the one stated above are that the set of thresholds $\mathcal{T}$ is closed and countable and that the eigenvalues of H can at most accumulate at $\mathcal{T}$. We discuss a third consequence, decay of non-threshold eigenstates, in Subsection 1.2.

1.2. **Generalized N-body hard-core systems.** The generalized hard-core model is a modification for the above model. For the generalized hard-core model we are given for each $a \in \mathcal{B}$ an open subset $\Omega_a \subset \mathbf{X}^a$ with $\mathbf{X}^a \setminus \Omega_a$ compact, possibly $\Omega_a = \mathbf{X}^a$. Let for $a_{\min} \neq b \subset a$

$$\Omega^a_b = \big(\Omega_b + \mathbf{X}_b\big) \cap \mathbf{X}^a = \Omega_b + \mathbf{X}_b \cap \mathbf{X}^a,$$

and for $a \neq a_{\min}$

$$\Omega^a = \cap_{a_{\min} \neq b \subset a} \Omega^a_b.$$

We define $\Omega^{a_{\min}} = \{0\}$ and $\Omega = \Omega^{a_{\max}}$.

Condition 1.4. There exists $\varepsilon > 0$ such that for all $b \in \mathcal{B}$ there is a splitting $V_b = V_b^{(1)} + V_b^{(2)}$, where

(1) $V_b^{(1)}$ is smooth on the closure of Ω_b and

$$\partial_y^\alpha V_b^{(1)}(y) = O\big(|y|^{-\varepsilon - |\alpha|}\big). \tag{1.8}$$

(2) $V_b^{(2)}$ vanishes outside a bounded set in Ω_b and

$$V_b^{(2)} \in \mathcal{C}\big(H_0^1(\Omega_b), H_0^1(\Omega_b)^*\big). \tag{1.9}$$

Here and henceforth, given Banach spaces X_1 and X_2, the notation $\mathcal{C}\big(X_1, X_2\big)$ and $\mathcal{B}\big(X_1, X_2\big)$ refers to the set of compact and the set of bounded operators $T : X_1 \to X_2$, respectively.

We consider for $a \in \mathcal{B}$ the Hamiltonian $H^a = -\frac{1}{2}\Delta_{x^a} + V^a$ on $L^2(\Omega^a)$ with Dirichlet boundary condition on $\partial\Omega^a$, in particular $H = \frac{1}{2}p^2 + V$ on $L^2(\Omega)$ with Dirichlet boundary condition on $\partial\Omega$. The corresponding form domain is the Sobolev space $H^1_0(\Omega^a)$. Due to the continuous embedding $H^1_0(\Omega^a) \subset H^1_0(\Omega^a_b)$ for $a_{\min} \neq b \subset a$ we conclude that indeed H^a is self-adjoint, cf. [RS, Theorem X.17]. Again we define $H^{a_{\min}} = 0$, and the set of thresholds is also given as in Subsection 1.1. We note that one can replace the Hilbert space $L^2(\mathbf{X})$ in Lemma 1.3 by $\mathcal{H} := L^2(\Omega)$ and then obtain a Mourre estimate for the present Hamiltonian H, cf. [Gri, Theorem 2.4]. All what is needed for this is to make sure that $R > 1$ is so large that the rescaled Graf vector field ω_R is complete on Ω. The latter is doable due to Lemma 1.2 (2) and (5).

According to [Gri, Theorem 2.5(1)] non-threshold eigenstates decay exponentially at rates determined by thresholds above the corresponding eigenvalues. This is a consequence of the hard-core Mourre estimate by arguments similar to the ones of [FH] for usual N-body Hamiltonians. In [Gri] Griesemer states as an open problem absence of positive eigenvalues under an additional connectedness condition. This is the problem we shall address in the present paper. The pattern of proof of [FH] does not work except the following induction scheme: For $N = 1$ absence of positive eigenvalues follows from various papers (assuming that $\Omega \subset \mathbf{X}$ is connected), for example most recently [IS2]. For $N \geq 2$ we could suppose by induction that the result holds for sub-Hamiltonians, whence that there are no positive thresholds. Using the hard-core Mourre estimate in a similar way as for soft potentials [FH, Gri, IS2] we then deduce that an eigenstate with corresponding positive eigenvalue would decay super-exponentially, cf. [Gri, Theorem 2.5(1)]. This would be derived in terms of the potential function r discussed below. Whence for any such eigenstate ϕ (i.e. corresponding to a positive eigenvalue) we would have $\mathrm{e}^{\sigma r}\phi \in L^2(\Omega)$ for all $\sigma \geq 0$. Consequently what would remain to be shown for completing the induction argument is that super-exponentially decaying eigenstates vanish.

Although we are not able in general to implement the above scheme for showing absence of positive eigenvalues we show a partial result which reduces the problem to resolvent estimates for sub-system type Hamiltonians. Moreover we do in fact implement the scheme for $N = 2$ under additional conditions.

Condition 1.5. Suppose $N \geq 2$. For all $b \in \mathcal{B} \setminus \{a_{\max}\}$ with $\Omega_b \subsetneq \mathbf{X}^b$ the set $\Theta_b := \mathbf{X}^b \setminus \overline{\Omega_b} \neq \emptyset$ has smooth boundary $\partial\Theta_b = \partial\Omega_b$ and is strictly convex.

For the notion of strict convexity used in this paper we refer to Appendix B. Given Condition 1.5, by definition if $\Omega_b \subsetneq \mathbf{X}^b$, then $\dim \mathbf{X}^b \geq 2$. With minor modifications we could have allowed $\dim \mathbf{X}^b = 1$ in the definition of strict convexity and obtained the same results, however for convenience we prefer not to do that.

The main result of this paper is the following.

Theorem 1.6. *Suppose $N = 2$ and Conditions 1.4 and 1.5. Suppose that for all $b \in \mathcal{B} \setminus \{a_{\max}\}$ with $\Omega_b \subsetneq \mathbf{X}^b$ the term $V_b^{(2)} = 0$ while for all $b \in \mathcal{B} \setminus \{a_{\max}\}$ with $\Omega_b = \mathbf{X}^b$*

$$x^b \cdot \nabla V_b^{(2)}(x^b),\ (x^b \cdot \nabla)^2 V_b^{(2)}(x^b) \in \mathcal{C}\big(H^1(\mathbf{X}^b), H^1(\mathbf{X}^b)^*\big). \tag{1.10}$$

Suppose that any eigenstate of H vanishing at infinity must be zero (the unique continuation property). Then H does not have positive eigenvalues.

The unique continuation property is a well-studied subject, see for example [Ge, JK, RS, Wo]. It is valid for a large class of potential singularities given connectedness of Ω.

Corollary 1.7. *For $N = 2$ charged particles confined to the exterior of a bounded strictly convex obstacle $\Theta_1 \subset \mathbb{R}^d$ containing 0, $d \geq 2$, the corresponding Hamiltonian H given by* (1.1) *with Coulomb interactions $V_j^{\mathrm{ncl}}(y) = q_j q^{\mathrm{ncl}}|y|^{-1}$ and $V_{ij}^{\mathrm{elec}}(y) = q_i q_j |y|^{-1}$ does not have positive eigenvalues.*

Note for Corollary 1.7 that indeed $\Omega = (\Omega_1)^2 \setminus \{(x_1, x_2) \in (\mathbb{R}^d)^2 | x_1 = x_2\}$ is a connected subset of $\mathbb{R}^{2d}$ for $d \geq 2$ (which follows readily using that $\Omega_1 \subset \mathbb{R}^d$ is connected) and that the version of the unique continuation property of [RS] applies.

Another result of this paper is the following statement in which a technical condition stated in Section 2 enters.

Proposition 1.8. *Suppose $N \geq 2$ and Conditions 1.4 and 2.1. Suppose H does not have positive thresholds. Suppose that any eigenstate of H vanishing at infinity must be zero (the unique continuation property). Then H does not have positive eigenvalues.*

By imposing the analogous version of Condition 2.1 for sub-Hamiltonians as well as the unique continuation property for these operators and for H (in addition to Condition 1.4) we obtain that H does not have positive thresholds nor positive eigenvalues, cf. the scheme discussed above. However since we are only able to verify Condition 2.1 for $N = 2$ using Condition 1.5 we need these restrictions in Theorem 1.6. Nevertheless, since verifying Condition 2.1 for higher N under Condition 1.4 possibly as well as under Condition 1.5 could be a purely technical difficulty, we consider Proposition 1.8 as a result of independent interest. We devote Section 2 to the crucial step in the proof. Section 3 is devoted to the verification of Condition 2.1 for $N = 2$. Supplementary material is given in Appendices A and B.

1.3. Geometric properties.

We complete this section by a brief discussion of some properties related to Lemma 1.2, and we show an estimate which may be viewed as a first step in a proof of (a hard-core version of) Lemma 1.3 (not to be elaborated on in this paper). These properties will be important in Section 2.

1.3.1. *Potential function.* Since ω_* is symmetric we can write

$$\omega = \nabla r^2/2.$$

It will be important for us that the function $r = r(x)$ can be chosen positive, smooth and convex, see the proof of [De, Proposition 4.4] (we remark that [De] also uses the Graf construction although with a different regularization procedure). From the convexity of r we learn that

$$\partial^r |\mathrm{d}r|^2 \geq 0;\ \partial^r f = \mathrm{i}p^r f := \nabla r \cdot \nabla f. \tag{1.11a}$$

We have a slight extension of part of (1.5), cf. [De, Lemma 4.3 f)],

$$\forall \alpha \in \mathbb{N}_0^{\dim \mathbf{X}} \text{ and } k \in \mathbb{N}_0 : |\partial_x^\alpha (x \cdot \nabla)^k \big(r^2 - x^2\big)| \leq C_\alpha. \tag{1.11b}$$

In particular we obtain yet another useful property

$$\forall \alpha \in \mathbb{N}_0^{\dim \mathbf{X}} : |\partial_x^\alpha \big(|\mathrm{d}r|^2 - 1\big)| \leq C_\alpha \langle x \rangle^{-2}. \tag{1.11c}$$

In fact letting $f = r^2 - x^2$ the bounds (1.11c) follow from (1.11b) and the identity

$$|\mathrm{d}r|^2 - 1 = \frac{x \cdot \nabla f + 4^{-1}|\mathrm{d}f|^2 - f}{x^2 + f}.$$

The rescaled r reads

$$r_R(x) = Rr(x/R),$$

so that $\omega_R = \nabla r_R^2/2$. Clearly the bounds (1.11a)-(1.11c) are also valid for the rescaled r (possibly with R-dependent constants). We also rescale the partition functions of Lemma 1.2 $\tilde{q}_{a,R}(x) := \tilde{q}_a(x/R)$ and similarly for the "quadratic" partition functions

$$q_b(x) = \tilde{q}_b(kx)\big(\sum_c \tilde{q}_c(kx)^2\big)^{-1/2};\ k = r_1/r_2.$$

Using that

$$\tilde{q}_c(x)\tilde{q}_b(kx) = 0 \text{ if } c \not\subset b,$$

and Lemma 1.2 (1) we conclude that

$$\omega_*(x) \geq \sum_b \pi_b q_b^2(x). \tag{1.12}$$

1.3.2. *Commutator calculation.* We calculate

$$\mathrm{i}[H, A_R] = 2p\omega_*(x/R)p - (4R^2)^{-1}\big(\Delta^2 r^2\big)(x/R) - 2\omega_R \cdot \nabla V, \tag{1.13}$$

and using (1.12) we thus deduce

$$\begin{aligned}\mathrm{i}[H, A_R] &\geq 2\sum_b q_{b,R}\, p_b^2\, q_{b,R} + O\big(R^{-2}\big) - 2\omega_R \cdot \nabla V\\ &= 2\sum_b q_{b,R}\, p_b^2\, q_{b,R} + O\big(R^{-\min\{2,\varepsilon\}}\big).\end{aligned} \tag{1.14}$$

1.3.3. *More notation.* We fix a non-negative $\chi \in C^\infty(\mathbb{R})$ with $0 \leq \chi \leq 1$ and

$$\chi(t) = \begin{cases} 0 & \text{for } t \leq 5/4, \\ 1 & \text{for } t \geq 7/4. \end{cases}$$

We shall frequently use the rescaled function

$$\chi_\nu(t) = \chi(t/\nu), \quad \nu > 0, \tag{1.15}$$

and the notation $\chi_\nu^+ = \chi_\nu$ and $\chi_\nu^- = \bar{\chi}_\nu = 1 - \chi_\nu$.

For any self-adjoint operator T and state ϕ we write $\langle T\rangle_\phi = \langle \phi, T\phi\rangle$ for the corresponding expectation value.

2. Reduction to high-energy hard-core sub-system resolvent bounds

Under Condition 1.4 we propose a scheme for showing

$$(H - E)\phi = 0,\ E > 0,\ \text{and } \forall \sigma \geq 0 :\ \mathrm{e}^{\sigma r}\phi \in \mathcal{H} = L^2(\Omega) \Rightarrow \phi = 0. \tag{2.1}$$

Here and henceforth $r = r_R$ is the rescaled potential function. We suppress the dependence on R which is fixed (large) from this point. The proposed method relies on the unique continuation property and certain high-energy hard-core sub-system type resolvent bounds. The latter are stated in Condition 2.1 given below. Whence we give the crucial step of the proof Proposition 1.8.

2.1. **General scheme.** For ϕ given as in (2.1) we let for any $\nu \geq 1$ and $\sigma \geq 0$

$$\phi_\sigma = \phi_{\sigma,\nu} := \chi_\nu \mathrm{e}^{\sigma(r-4\nu)}\phi \in \mathcal{H};\ \chi_\nu = \chi_\nu(r). \tag{2.2}$$

Putting $H^\sigma = H - \frac{\sigma^2}{2}|\mathrm{d}r|^2$ we note that

$$(H^\sigma - E)\phi_\sigma = -\mathrm{i}\sigma(\mathrm{Re}\, p^r)\phi_\sigma - \mathrm{i}\mathrm{e}^{\sigma(r-4\nu)}R(\nu)\phi, \tag{2.3}$$

where $R(\nu) = \mathrm{i}[H_0, \chi_\nu] = \mathrm{Re}\,\big(\chi'_\nu p^r\big)$. Whence by undoing the commutator, cf. Appendix A,

$$\langle \mathrm{i}[H^\sigma, A]\rangle_{\phi_\sigma} = -2\sigma\,\mathrm{Re}\,\langle(\mathrm{Re}\, p^r)A\rangle_{\phi_\sigma} - 2\,\mathrm{Re}\,\langle R(\nu)\mathrm{e}^{\sigma(r-4\nu)}A\chi_\nu\mathrm{e}^{\sigma(r-4\nu)}\rangle_\phi. \tag{2.4}$$

The first term of (2.4) is computed

$$\begin{aligned} &-2\sigma\,\mathrm{Re}\,((\mathrm{Re}\, p^r)A)\\ &= -\sigma(\mathrm{Re}\, p^r)(2r\,\mathrm{Re}\, p^r - \mathrm{i}|\mathrm{d}r|^2) + \mathrm{h.c.}\\ &= -4\sigma(\mathrm{Re}\, p^r)r\,\mathrm{Re}\, p^r + \sigma(\partial^r|\mathrm{d}r|^2). \end{aligned} \tag{2.5}$$

As for the second term we estimate (recall the notation $\bar\chi_\nu = 1 - \chi_\nu$)

$$\begin{aligned} &-2\,\mathrm{Re}\,\langle R(\nu)\mathrm{e}^{\sigma(r-4\nu)}A\chi_\nu\mathrm{e}^{\sigma(r-4\nu)}\rangle_\phi\\ &\leq \|\mathrm{e}^{\sigma(r-4\nu)}R(\nu)\phi\|^2 + \|\bar\chi_{2\nu}A\chi_\nu\mathrm{e}^{\sigma(r-4\nu)}\phi\|^2\\ &\leq \big\{\|\chi'_\nu\mathrm{e}^{\sigma(r-4\nu)}p^r\phi\| + \tfrac12\|(\chi''_\nu|\mathrm{d}r|^2 + \chi'_\nu(\Delta r))\mathrm{e}^{\sigma(r-4\nu)}\phi\|\big\}^2\\ &\quad + \big\{\|2r\bar\chi_{2\nu}\chi_\nu\mathrm{e}^{\sigma(r-4\nu)}p^r\phi\| + \|\bar\chi_{2\nu}(2r|\mathrm{d}r|^2\chi'_\nu + 2\sigma r\chi_\nu|\mathrm{d}r|^2 + \tfrac12(\Delta r^2)\chi_\nu)\mathrm{e}^{\sigma(r-4\nu)}\phi\|\big\}^2\\ &\leq C\nu^2\|\chi_{\nu/2}|p\phi|\|^2 + C\nu^2\langle\sigma\rangle^2\|\phi\|^2\\ &\leq C\nu^2\langle p^2\rangle_\phi + C\nu^2\langle\sigma\rangle^2\|\phi\|^2. \end{aligned}$$

Note that $C > 0$ does not depend on ν or σ because $r \leq 2\nu$ on $\mathrm{supp}\,\chi'_\nu$. Using the relative ϵ-smallness of the potential we have for some $C > 0$

$$\langle p^2\rangle_\phi \leq \langle 4H + C\rangle_\phi = (4E + C)\|\phi\|^2, \tag{2.6}$$

and we deduce that

$$-2\,\mathrm{Re}\,\langle R(\nu)\mathrm{e}^{\sigma(r-4\nu)}A\chi_\nu\mathrm{e}^{\sigma(r-4\nu)}\rangle_\phi \leq C\nu^2\langle\sigma\rangle^2\|\phi\|^2. \tag{2.7}$$

On the other hand doing the commutator, cf. (1.13), and then using (1.11a) and (1.14) we obtain that

$$\begin{aligned} \langle \mathrm{i}[H^\sigma, A]\rangle_{\phi_\sigma} &\geq -\sigma^2\mathrm{Im}\,\langle A|\mathrm{d}r|^2\rangle_{\phi_\sigma} + 2\sum_b\langle p_b^2\rangle_{q_{b,R}\phi_\sigma} - o(R^0)\|\phi_\sigma\|^2\\ &= \sigma^2\langle r\partial^r|\mathrm{d}r|^2\rangle_{\phi_\sigma} + 2\sum_b\langle p_b^2\rangle_{q_{b,R}\phi_\sigma} - o(R^0)\|\phi_\sigma\|^2\\ &\geq \sigma\langle\partial^r|\mathrm{d}r|^2\rangle_{\phi_\sigma} + 2\sum_b\langle p_b^2\rangle_{q_{b,R}\phi_\sigma} - o(R^0)\|\phi_\sigma\|^2 \end{aligned} \tag{2.8}$$

We combine (2.4)–(2.8) and conclude that

$$\begin{aligned} &C\nu^2\langle\sigma\rangle^2\|\phi\|^2 + o(R^0)\|\phi_\sigma\|^2\\ &\quad\geq 4\sigma\langle r\rangle_{(\mathrm{Re}\, p^r)\phi_\sigma} + 2\sum_b\langle p_b^2\rangle_{q_{b,R}\phi_\sigma}. \end{aligned} \tag{2.9}$$

We aim at deriving some useful positivity from the second term of (2.9) to the right. For that let us for $b \in \mathcal{A}$ introduce

$$\begin{aligned}\widetilde{H}_b &= \widetilde{H}^b + \tilde{p}_b^2 \chi^-_{\sigma^2/2}\big(\tilde{p}_b^2\big); \qquad (2.10)\\ \widetilde{H}^b &= s(x)^{-1} H^b s(x)^{-1},\ \tilde{p}_b^2 = \tfrac12 s(x)^{-1} p_b^2 s(x)^{-1} \text{ where}\\ s(x) &= \chi^+_{\nu/2}(r)(|\mathrm{d}r|-1)/\sqrt{2} + 1/\sqrt{2}.\end{aligned}$$

Here we suppressed the dependence of $\widetilde{H}_b$ on the parameter R (through r, and considered as fixed) as well as the dependence on ν and σ. The latter parameters will be considered as independent large parameters (at the end we fix ν large and let $\sigma \to \infty$). The operator $\widetilde{H}_b - \sigma^2$ should be thought of as an effective approximation to

$$2|\mathrm{d}r|^{-1}\big(H_b - \tfrac{\sigma^2}{2}|\mathrm{d}r|^2\big)|\mathrm{d}r|^{-1} \approx 2H_b - \sigma^2 = 2H^b + p_b^2 - \sigma^2.$$

Let us here note the following consequence of (1.11c)

$$\forall \alpha \in \mathbb{N}_0^{\dim \mathbf{X}} : |\partial_x^\alpha\big(s(x) - 1/\sqrt{2}\big)| \le C_\alpha \nu^{-2}. \qquad (2.11)$$

The definitions (2.10) are accompanied by the following specification of domains: For $b \in \mathcal{A}$ we define

$$\mathcal{H}_b = L^2(\Omega^b) \otimes L^2(\mathbf{X}_b) = L^2(\Omega^b + \mathbf{X}_b),$$

and note that

$$\mathcal{H}_b \subset L^2(\mathbf{X}^b) \otimes L^2(\mathbf{X}_b) = L^2(\mathbf{X}).$$

The first term of (2.10), $\widetilde{H}^b$, is an operator on $\mathcal{H}_b$. We specify its form domain to be $L^2(\mathbf{X}_b, H_0^1(\Omega^b); \mathrm{d}x_b)$. The corresponding quadratic form is closed. The operator $\tilde{p}_b^2$ is an operator on $L^2(\mathbf{X})$ with $Q(\tilde{p}_b^2) = Q(p_b^2) = L^2(\mathbf{X}^b) \otimes H^1(\mathbf{X}_b)$ and $\mathcal{D}(\tilde{p}_b^2) = \mathcal{D}(p_b^2) = L^2(\mathbf{X}^b) \otimes H^2(\mathbf{X}_b)$. However since it is multiplicative in the x^b variable the space $\mathcal{H}_b$ is an invariant subspace, in fact $\mathcal{D}(\tilde{p}_b^2) \cap \mathcal{H}_b = L^2(\Omega^b) \otimes H^2(\mathbf{X}_b)$. Whence clearly the second term of (2.10) is a bounded operator on $\mathcal{H}_b$ (with the norm bound $\frac78\sigma^2$). We conclude $\widetilde{H}_b$ is a well-defined operator on $\mathcal{H}_b$ with form domain

$$Q(\widetilde{H}_b) = L^2(\mathbf{X}_b, H_0^1(\Omega^b); \mathrm{d}x_b) \subset \mathcal{H}_b.$$

For later applications let us note the facts that $\mathcal{D}(\tilde{p}_c^2) \supset \mathcal{D}(\tilde{p}_b^2)$ and $\mathcal{H}_b \supset \mathcal{H}_c$ for all $c \supset b$ (the latter embedding is due to the relation $\Omega^b + \mathbf{X}_b \supset \Omega^c + \mathbf{X}_c$).

We introduce a technical condition for the operators introduced in (2.10).

Condition 2.1. For all $b \neq a_{\max}$ the following bound holds uniformly in all large $\sigma, \nu > 1$, $\epsilon \in (0, 1]$ and reals λ near 1:

$$\|\delta_\epsilon(\widetilde{H}_b/\sigma^2 - \lambda)\|_{\mathcal{B}(B(|x^b|), B(|x^b|)^*)} \le C\sigma. \qquad (2.12)$$

Here, by definition, for any self-adjoint operator T

$$\delta_\epsilon(T) = \pi^{-1} \mathrm{Im}\,(T - \mathrm{i}\epsilon)^{-1}.$$

The space $B(\cdot)$ is a Besov space, see Subsection 3.1 for the abstract definition. Note that (2.12) is trivially fulfilled for $b = a_{\min}$ (by the spectral theorem). We derive the bounds for $N = 2$ in Section 3 under the additional regularity conditions on the obstacles and potentials stated in Theorem 1.6. Note that for $N = 2$ and $b \notin \{a_{\min}, a_{\max}\}$ only $b' = b$ obeys $a_{\min} \neq b' \subset b$, and hence for such b we have

$\Omega^b = \Omega_b$ and (2.12) is an effective high energy bound for a bounded obstacle (hence one-body type). More generally we prove (2.12) for b with $\#b = N$ under the additional regularity conditions for Ω_b and V_b. High energy resolvent bounds are studied previously in the literature, see for example [Je, Vo1, Vo2, RT]. Although slightly weaker bounds than (2.12) will suffice (Besov spaces can be replaced by weighted spaces for example) we need the linear dependence of σ on the right hand side. Whence the slightly weaker dependence $\sigma \ln \sigma$ found in recent works on one-body obstacle problems (see for example [Chr]) would not suffice.

Let us also introduce $\tilde{\phi}_\sigma = s(x)\phi_\sigma$. We estimate for $b \neq a_{\max}$, $k_1 > 0$ (can be fixed arbitrarily) and all large $\sigma > 1$

$$\begin{aligned} \tfrac{1}{2}\langle p_b^2\rangle_{q_{b,R}\phi_\sigma} &= \langle \tilde{p}_b^2\rangle_{q_{b,R}\tilde{\phi}_\sigma} \\ &\geq \langle \tilde{p}_b^2 \chi^+_{k_1\sigma}\big(\tilde{p}_b^2\big)\rangle_{q_{b,R}\tilde{\phi}_\sigma} \\ &\geq k_1\sigma\big(\|q_{b,R}\tilde{\phi}_\sigma\|^2 - \langle \chi^-_{k_1\sigma}\big(\tilde{p}_b^2\big)\rangle_{q_{b,R}\tilde{\phi}_\sigma}\big) \\ &\geq k_1\sigma\big(\|q_{b,R}\tilde{\phi}_\sigma\|^2 - \langle \chi^-_{\sigma^2/8}\big(\tilde{p}_b^2\big)\rangle_{q_{b,R}\tilde{\phi}_\sigma}\big). \end{aligned} \tag{2.13}$$

The contribution to (2.9) from the first term to the right in (2.13) amounts (for $\nu \geq Rr_2$) to the positive term $4k_1\sigma\|\tilde{\phi}_\sigma\|^2$, and it remains to estimate the contribution from the second term to the right. Now up to a term of order $O(\sigma^{-2})$ better it is given by summing the expressions $-4k_1\sigma \mathrm{Re}\,\langle \chi^-_{\sigma^2/8}\big(\tilde{p}_b^2\big) q_{b,R}^2\rangle_{\tilde{\phi}_\sigma}$.

We write for $b \neq a_{\max}$ and $R_1 \geq Rr_2/r_1$

$$q_{b,R}^2 = q_{b,R}^2 \sum_{b_1 \supset b} q_{b_1,R_1}^2 = q_{b,R}^2 q_{b,R_1}^2 + q_{b,R}^2 \sum_{b_1 \supsetneq b} q_{b_1,R_1}^2.$$

Actually we shall later need $R_1 >> R$. We repeat the expansion by writing for $R_2 >> R_1$ and $b_1 \supsetneq b$

$$q_{b,R}^2 q_{b_1,R_1}^2 = q_{b,R}^2 q_{b_1,R_1}^2 q_{b_1,R_2}^2 + \sum_{b_2 \supsetneq b_1} q_{b,R}^2 q_{b_1,R_1}^2 q_{b_2,R_2}^2.$$

Upon further iteration the procedure stops for each branch after say n times when necessarily $b_n = a_{\max}$ (n is at most N). Whence the only non-trivial terms to examine have the form

$$q_{b,R}^2 q_{b,R_1}^2 \text{ or } q_{b,R}^2 \prod_{1\leq j\leq m} q_{b_j,R_j}^2 q_{b_m,R_{m+1}}^2,$$

where $m \leq n-1$, $b \subsetneq b_1 \cdots \subsetneq b_m \subsetneq a_{\max}$ and $R << R_1 \cdots << R_m << R_{m+1}$. As the reader will see these constraints are needed later, see the verification of (2.20). Moreover we shall need the constraint $\nu \geq R_{m+1}r_2$. Introducing the notation $b_0 = b$ and $R_0 = R$ in either case the form is then $q_{b_m,R_m}^2 q_{b_m,R_{m+1}}^2$ times a bounded factor Q_m^2, in fact $|Q_m(x)| \leq 1$. We decompose

$$\begin{aligned} &\mathrm{Re}\,\big(\chi^-_{\sigma^2/8}\big(\tilde{p}_b^2\big) q_{b,R}^2\big) \\ &= \mathrm{Re}\,\big(\sum \chi^-_{\sigma^2/8}\big(\tilde{p}_b^2\big) q_{b_m,R_m}^2 q_{b_m,R_{m+1}}^2 Q_m^2\big) + \mathrm{Re}\,\big(\sum \chi^-_{\sigma^2/8}\big(\tilde{p}_b^2\big) q_{b_m,R_m}^2 q_{a_{\max},R_{m+1}}^2 Q_m^2\big) \\ &= \sum q_{b_m,R_{m+1}} q_{b_m,R_m} Q_m \chi^-_{\sigma^2/8}\big(\tilde{p}_b^2\big) Q_m q_{b_m,R_m} q_{b_m,R_{m+1}} + \text{ remainder.} \end{aligned}$$

Here the remainder is the sum of terms either $O(\sigma^{-2})$ better than "the good term" $4k_1\sigma\|\tilde{\phi}_\sigma\|^2$ we derived from (2.13) or being expressed by factors of $q_{a_{\max},R_{m+1}}$. Whence (using $\nu \geq R_{m+1}r_2$) the remainder conforms with (2.9).

Next on both sides of the factor $\chi^-_{\sigma^2/8}(\tilde p_b^2)$ in the summation to the right we insert

$$I = \chi^-_{\sigma^2/4}(\tilde p_{b_m}^2) + \chi^+_{\sigma^2/4}(\tilde p_{b_m}^2).$$

This yields four times as many terms. The contribution from the terms with two factors of $\chi^-_{\sigma^2/4}$ is then estimated as

$$\begin{aligned}&\sum q_{b_m,R_{m+1}} q_{b_m,R_m} Q_m \chi^-_{\sigma^2/4}(\tilde p_{b_m}^2)\chi^-_{\sigma^2/8}(\tilde p_b^2)\chi^-_{\sigma^2/4}(\tilde p_{b_m}^2) Q_m q_{b_m,R_m} q_{b_m,R_{m+1}}\\ &\leq \mathrm{Re}\Big(\sum q^2_{b_m,R_{m+1}}\chi^-_{\sigma^2/4}(\tilde p_{b_m}^2)^2 q^2_{b_m,R_m} Q_m^2\Big) + O(\sigma^{-2}).\end{aligned} \tag{2.14}$$

We take a closer look at the first term later. We first consider the contributions from

$$2\mathrm{Re}\Big(\chi^+_{\sigma^2/4}(\tilde p_{b_m}^2)\chi^-_{\sigma^2/8}(\tilde p_b^2)\chi^-_{\sigma^2/4}(\tilde p_{b_m}^2)\Big) + \chi^+_{\sigma^2/4}(\tilde p_{b_m}^2)\chi^-_{\sigma^2/8}(\tilde p_b^2)\chi^+_{\sigma^2/4}(\tilde p_{b_m}^2).$$

For this purpose let us for $\psi \in L^2(\mathbf{X})$ introduce

$$\psi_\sigma = \chi^+_{\sigma^2/4}(\tilde p_{b_m}^2)\chi^-_{\sigma^2/8}(\tilde p_b^2)\psi \text{ and } \widetilde\psi_\sigma = \chi^-_{\sigma^2/8}(\tilde p_b^2)\chi^+_{\sigma^2/4}(\tilde p_{b_m}^2)\psi.$$

We apply (see below for a proof)

$$\|[\chi^+_{\sigma^2/4}(\tilde p_{b_m}^2), \chi^-_{\sigma^2/8}(\tilde p_b^2)]\| \leq C\tfrac{1}{\sigma\nu}, \tag{2.15a}$$

yielding

$$\|\psi_\sigma - \widetilde\psi_\sigma\| \leq C\tfrac{1}{\sigma\nu}\|\psi\|,$$

and whence with the operator monotone function $f(t) = (t-1)/(1+t)$

$$\begin{aligned}\|\widetilde\psi_\sigma\|^2 &\leq 2\|\psi_\sigma\|^2 + C\tfrac{1}{\sigma^2\nu^2}\|\psi\|^2\\ &\leq 2f(\tfrac54)^{-1}\langle f(\tfrac{4}{\sigma^2}\tilde p_{b_m}^2)\rangle_{\psi_\sigma} + C\tfrac{1}{\sigma^2\nu^2}\|\psi\|^2\\ &\leq 2f(\tfrac54)^{-1}\langle f(\tfrac{4}{\sigma^2}\tilde p_b^2)\rangle_{\psi_\sigma} + C\tfrac{1}{\sigma^2\nu^2}\|\psi\|^2.\end{aligned}$$

Obviously it follows from (2.15a) that

$$\|f(\tfrac{4}{\sigma^2}\tilde p_b^2)[\chi^+_{\sigma^2/4}(\tilde p_{b_m}^2), \chi^-_{\sigma^2/8}(\tilde p_b^2)]\| \leq C\tfrac{1}{\sigma\nu}, \tag{2.15b}$$

and we can "reverse the commutation"

$$\begin{aligned}&2f(\tfrac54)^{-1}\langle f(\tfrac{4}{\sigma^2}\tilde p_b^2)\rangle_{\psi_\sigma}\\ &\quad\leq 2f(\tfrac54)^{-1}\langle f(\tfrac{4}{\sigma^2}\tilde p_b^2)\rangle_{\widetilde\psi_\sigma} + C\tfrac{1}{\sigma\nu}\|\psi\|\,\|\psi_\sigma\| + C\tfrac{1}{\sigma\nu}\|\psi\|\,\|\widetilde\psi_\sigma\|\\ &\quad\leq 2f(\tfrac54)^{-1}f(\tfrac78)\|\widetilde\psi_\sigma\|^2 + \|\psi_\sigma\|^2 + \epsilon\|\widetilde\psi_\sigma\|^2 + C_\epsilon\tfrac{1}{\sigma^2\nu^2}\|\psi\|^2\\ &\quad\leq \|\psi_\sigma\|^2 + C_\epsilon\tfrac{1}{\sigma^2\nu^2}\|\psi\|^2;\end{aligned}$$

here we took $\epsilon = 2f(\tfrac54)^{-1}|f(\tfrac78)|$, for example. By combining with the previous estimation we find

$$\|\psi_\sigma\|^2 \leq C\tfrac{1}{\sigma^2\nu^2}\|\psi\|^2,$$

and then in turn

$$\|\psi_\sigma\|,\ \|\widetilde\psi_\sigma\| \leq C\tfrac{1}{\sigma\nu}\|\psi\|.$$

We conclude that indeed, due to errors of the form $O(\nu^{-1}\sigma^{-1}) + O(\sigma^{-2})$, we need to examine the first term of (2.14) only.

2.1.1. *Verification of* (2.15a). Introduce $P_m = \sigma^{-2}\tilde p_{b_m}^2$ and $P = \sigma^{-2}\tilde p_b^2$. We show the slightly stronger bound

$$\|[\chi^+_{1/4}(P_m), \chi^-_{1/8}(P)]\| = \|[\chi^-_{1/4}(P_m), \chi^-_{1/8}(P)]\| \le C\tfrac{1}{\sigma\nu^2}. \tag{2.15c}$$

Since $P_m, P \ge 0$ we can truncate χ^-_ν, $\nu = 1/4, 1/8$, at the negative half-axis to become functions χ_1, χ_2 in $C_c^\infty(\mathbb{R})$ and invoke the standard representation for a self-adjoint operator T and such function χ

$$\chi(T) = \int_{\mathbb{C}} (T-z)^{-1}\, \mathrm{d}\mu(z),\ \mathrm{d}\mu(z) = -\frac{1}{2\pi\mathrm{i}}\bar\partial\tilde\chi(z)\mathrm{d}z\mathrm{d}\bar z, \tag{2.16}$$

where we have used an almost analytic extension $\tilde\chi \in C_c^\infty(\mathbb{C})$, i.e.

$$\tilde\chi(t) = \chi(t) \text{ for } t \in \mathbb{R}, \qquad |\bar\partial\tilde\chi(z)| \le C_k|\operatorname{Im} z|^k;\ k \in \mathbb{N}.$$

Whence

$$\chi^-_{1/4}(P_m) = \int_{\mathbb{C}} (P_m - z_1)^{-1}\, \mathrm{d}\mu_1(z_1), \tag{2.17a}$$

$$\chi^-_{1/8}(P) = \int_{\mathbb{C}} (P - z_2)^{-1}\, \mathrm{d}\mu_2(z_2). \tag{2.17b}$$

Using (2.17a), (2.17b) and the domain relation $\mathcal{D}(P_m) \supset \mathcal{D}(P)$ we represent

$$[\chi^-_{1/4}(P_m), \chi^-_{1/8}(P)] = \int_{\mathbb{C}}\int_{\mathbb{C}} (P_m - z_1)^{-1}(P-z_2)^{-1} [P_m, P](P-z_2)^{-1}(P_m - z_1)^{-1}\, \mathrm{d}\mu_2(z_2)\mathrm{d}\mu_1(z_1).$$

Next we note the elementary bounds

$$\|(P_m - z)^{-1}\| \le \tfrac{1}{|\operatorname{Im} z|}, \tag{2.18a}$$

$$\|\langle P\rangle (P-z)^{-1}\| \le C\tfrac{|z|+1}{|\operatorname{Im} z|}. \tag{2.18b}$$

Using (2.11) we compute

$$\|\langle P\rangle^{-1}[P_m, P]\langle P\rangle^{-1}\| \le C\tfrac{1}{\sigma\nu^2}. \tag{2.18c}$$

Finally applying (2.18a)–(2.18c) to the double integral we obtain the bound

$$\cdots \le C_1\tfrac{1}{\sigma\nu^2}\int_{\mathbb{C}}\int_{\mathbb{C}} |\operatorname{Im} z_1|^{-2}\tfrac{(|z_2|+1)^2}{|\operatorname{Im} z_2|^2}\, |\mathrm{d}\mu_2(z_2)|\, |\mathrm{d}\mu_1(z_1)| = C_2\tfrac{1}{\sigma\nu^2},$$

and we have shown (2.15c).

2.1.2. *Localization for first term of* (2.14). We decompose (for $k_2 > 0$ to be fixed later, big)

$$q^2_{b_m,R_{m+1}}\chi^-_{\sigma^2/4}\big(\tilde p^2_{b_m}\big)^2 q^2_{b_m,R_m}Q_m^2 = q^2_{b_m,R_{m+1}}\chi^-_{\sigma^2/4}\big(\tilde p^2_{b_m}\big)(\chi^- + \chi^+)q^2_{b_m,R_m}Q_m^2;$$
$$\chi^- := \chi^-_{(k_2R_m\sigma)^{-1}}(|\widetilde H_{b_m}/\sigma^2 - 1|),$$
$$\chi^+ := \chi^+_{(k_2R_m\sigma)^{-1}}(|\widetilde H_{b_m}/\sigma^2 - 1|).$$

To treat the contribution from χ^- we write $q^2_{b_m,R_m} = \chi^-_{r_2R_m}(|x^{b_m}|)q^2_{b_m,R_m}$. Now imposing Condition 2.1 and applying (2.12) with $b = b_m$ we get using

$$\|\chi^-_{r_2R_m}(|x^{b_m}|)\|_{\mathcal{B}(\mathcal{H}_{b_m}, B(|x^{b_m}|))} \le C\sqrt{r_2R_m}$$

that

$$\|\chi^-_{r_2R_m}(|x^{b_m}|)(\chi^-)^2\chi^-_{r_2R_m}(|x^{b_m}|)\|_{\mathcal{B}(\mathcal{H}_{b_m})} \le C_1/k_2. \tag{2.19}$$

Here we used the general bound for S bounded and T self-adjoint

$$\|S^* g(T) S\| \leq \|g\|_{L^1} \sup_{\lambda \in \operatorname{supp} g, \epsilon \in (0,1]} \|S^* \delta_\epsilon (T - \lambda) S\|,$$

cf. Stone's formula [RS]. We fix k_2 such that $(\#\mathcal{A})^{N+1}\sqrt{C_1/k_2} \leq 1/2$, saving "the good term" $2k_1\sigma\|\tilde{\phi}_\sigma\|^2$ in the previous bound (2.9).

2.1.3. *Completion of proof of* (2.1). We need to examine the contribution from χ^+ to (2.9). We write

$$q^2_{b_m,R_{m+1}}\chi^-_{\sigma^2/4}\big(\tilde{p}^2_{b_m}\big)^2\chi^+ = k_2 R_m \sigma q^2_{b_m,R_{m+1}}\chi^-_{\sigma^2/4}\big(\tilde{p}^2_{b_m}\big)^2\big(\widetilde{H}_{b_m}/\sigma^2 - 1\big)\widetilde{Q}_m,$$

where $\widetilde{Q}_m = \widetilde{Q}_m(\widetilde{H}_{b_m}/\sigma^2)$ is bounded with norm at most 1. Taking expectation in $\tilde{\phi}_\sigma$ and using the Cauchy Schwarz inequality it suffices to bound

$$\begin{aligned} &4k_1\sigma \sum k_2 R_m \sigma^{-1} \|(\widetilde{H}_{b_m} - \sigma^2)\chi^-_{\sigma^2/4}\big(\tilde{p}^2_{b_m}\big)^2 q^2_{b_m,R_{m+1}}\tilde{\phi}_\sigma\|\,\|\tilde{\phi}_\sigma\| \\ &\leq k_1\sigma\|\tilde{\phi}_\sigma\|^2 + 4\sigma\langle r\rangle_{(\operatorname{Re} p^r)\phi_\sigma} + C\big(\nu^2\langle\sigma\rangle^2\|\phi\|^2 + \|\phi_\sigma\|^2\big). \end{aligned} \tag{2.20}$$

With (2.9) this yields

$$C\big(\nu^2\langle\sigma\rangle^2\|\phi\|^2 + \|\phi_\sigma\|^2\big) \geq k_1\sigma\Big(1 - O\big(\nu^{-1}\sigma^{-1}\big) - O\big(\sigma^{-2}\big)\Big)\|\tilde{\phi}_\sigma\|^2,$$

and we learn by letting $\sigma \to \infty$ that $\chi_{4\nu}(r)\phi \equiv 0$ (for ν large), and then in turn from the unique continuation property that $\phi = 0$.

2.1.4. *Mapping properties.* As a preparation for proving (2.20) let us note the following mapping properties of $S = \chi^-_{\sigma^2/4}\big(\tilde{p}^2_a\big)^2$ and $T = q^2_{a,R_{m+1}}$ entering in (2.20) with $a = b_m$. Recall that the form domain $Q\big(\widetilde{H}_a\big)$ of $\widetilde{H}_a$ is $L^2(\mathbf{X}_a, H^1_0(\Omega^a); \mathrm{d}x_a)$.

$$S \in \mathcal{B}\big(Q\big(\widetilde{H}_a\big), H^1_0(\Omega^a + \mathbf{X}_a)\big), \tag{2.21a}$$

$$T \in \mathcal{B}\big(H^1_0(\Omega^a + \mathbf{X}_a), H^1_0(\Omega)\big), \tag{2.21b}$$

$$TS \in \mathcal{B}\big(Q\big(\widetilde{H}_a\big), H^1_0(\Omega)\big), \tag{2.21c}$$

$$TS \in \mathcal{B}\big(Q\big(\widetilde{H}_a\big)\big). \tag{2.21d}$$

For (2.21a) we can use (2.16) to represent $S = \chi\big(\tilde{p}^2_a\big)$, apply the integral to a simple tensor $\psi^a \otimes \psi_a$ and then calculate derivatives of the resulting expression (not to be elaborated on). Clearly S is a smoothing operator in the x_a variable yielding the improved smoothness. Also we note that since S is multiplicative in the x^a variable it preserves the support in this variable of elements of an approximating sequence. We obtain that indeed $S\psi_a \otimes \psi^a \in H^1_0(\Omega^a + \mathbf{X}_a)$ with

$$\|S\psi^a \otimes \psi_a\|_1 \leq C\|\psi^a \otimes \psi_a\|_{Q(\widetilde{H}_a)}.$$

This bound extends to finite sums of simple tensors (by the same arguments) and hence (2.21a) follows by density and continuity. As for (2.21b) we use that

$$\operatorname{supp}\big(q^2_{a,R_{m+1}}\big) \cap \big(\Omega^a + \mathbf{X}_a\big) \subset \Omega.$$

Clearly (2.21c) follows from (2.21a) and (2.21b), while in turn (2.21d) follows from (2.21c) and the inclusion $\Omega \subset \Omega^a + \mathbf{X}_a$ implying that $H^1_0(\Omega)$ is continuously embedded in $H^1_0(\Omega^a + \mathbf{X}_a)$ and therefore in $Q\big(\widetilde{H}_a\big)$.

2.1.5. *Proof of* (2.20). We consider the vector $(\widetilde{H}_a-\sigma^2)\chi^-_{\sigma^2/4}\big(\tilde{p}_a^2\big)^2 q^2_{a,R_{m+1}}\tilde{\phi}_\sigma$, $a=b_m$, in (2.20) as an element of the dual space of the form domain $Q\big(\widetilde{H}_a\big)$, that is in $L^2(\mathbf{X}_a, H^1_0(\Omega^a)^*; \mathrm{d}x_a)$. As a part of (2.20) we must show that indeed it belongs to $\mathcal{H}_a$. This will follow from (2.21c) and the calculations below. We rewrite, using that $\tilde{\phi}_\sigma\in Q\big(\widetilde{H}_a\big)$, $\widetilde{H}_a\tilde{\phi}_\sigma\in Q\big(\widetilde{H}_a\big)^*$ and (2.21d),

$$(\widetilde{H}_a-\sigma^2)\chi^-_{\sigma^2/4}\big(\tilde{p}_a^2\big)^2 q^2_{a,R_{m+1}}\tilde{\phi}_\sigma=\chi^-_{\sigma^2/4}\big(\tilde{p}_a^2\big)^2 q^2_{a,R_{m+1}}(\widetilde{H}_a-\sigma^2)\tilde{\phi}_\sigma+T_{\mathrm{com}}$$
$$T_{\mathrm{com}}=[\widetilde{H}_a,\chi^-_{\sigma^2/4}\big(\tilde{p}_a^2\big)^2 q^2_{a,R_{m+1}}]\tilde{\phi}_\sigma,$$

and then

$$\begin{aligned}(\widetilde{H}_a-\sigma^2)\tilde{\phi}_\sigma&=s(x)^{-1}\big(\tfrac12 p_a^2 s(x)^{-1}\chi^-_{\sigma^2/2}\big(\tilde{p}_a^2\big)s(x)+H^a-\tfrac{\sigma^2}{2}|\mathrm{d}r|^2\big)\phi_\sigma\\&=s(x)^{-1}\big((H^\sigma-E+\mathrm{i}\sigma(\mathrm{Re}\,p^r))\phi_\sigma+\mathrm{i}\mathrm{e}^{\sigma(r-4\nu)}R(\nu)\phi\big)+T_1+T_2+T_3\\T_1&=-\tilde{p}_a^2\chi^+_{\sigma^2/2}\big(\tilde{p}_a^2\big)\tilde{\phi}_\sigma,\\T_2&=s(x)^{-1}\big(E-I_a-\mathrm{i}\sigma(\mathrm{Re}\,p^r)\big)\phi_\sigma\\T_3&=-s(x)^{-1}\mathrm{i}\mathrm{e}^{\sigma(r-4\nu)}R(\nu)\phi.\end{aligned}$$

Due to (2.3) (and (2.21c)) we need to estimate the contributions from T_1–T_3 and T_{com} only.

As for T_1 we note that $(\chi^-_{\sigma^2/4})^2\chi^+_{\sigma^2/2}=0$. Whence by commutation

$$\|\chi^-_{\sigma^2/4}\big(\tilde{p}_a^2\big)^2 q^2_{a,R_{m+1}}T_1\|\le C\tfrac{\sigma}{R_{m+1}}\|\tilde{\phi}_\sigma\|,$$

which agrees with (2.20) provided $R_{m+1}>>R_m$.

We estimate

$$\begin{aligned}\|\chi^-_{\sigma^2/4}\big(\tilde{p}_a^2\big)^2 q^2_{a,R_{m+1}}T_2\|^2&\le C\|\phi_\sigma\|^2+2\sigma^2\|(\mathrm{Re}\,p^r)\phi_\sigma\|^2\\&\le(C+O(\sigma^2/\nu^2))\|\phi_\sigma\|^2+\tfrac{2}{\nu}\sigma^2\langle r\rangle_{(\mathrm{Re}\,p^r)\phi_\sigma}.\end{aligned}$$

Whence the contribution from T_2 to the bound (2.20) is given by

$$\cdots\le C\epsilon^{-1}R_m\big((\sigma^{-1}+\tfrac{\sigma}{\nu^2})\|\phi_\sigma\|^2+\tfrac{\sigma}{\nu}\langle r\rangle_{(\mathrm{Re}\,p^r)\phi_\sigma}\big)+\epsilon R_m\sigma\|\tilde{\phi}_\sigma\|^2.$$

This bound agrees with (2.20) for all large ν and σ if we choose $\epsilon>0$ small (note that $\nu>>R_m$ is used). Notice that we needed the second term on the right hand side of (2.20) (this is the only occurrence).

As for the contribution from T_3 we invoke (2.6).

To treat the contribution from T_{com} we decompose

$$T_{\mathrm{com}}=\chi^-_{\sigma^2/4}\big(\tilde{p}_a^2\big)^2[\widetilde{H}_a,q^2_{a,R_{m+1}}]\tilde{\phi}_\sigma+[\widetilde{H}_a,\chi^-_{\sigma^2/4}\big(\tilde{p}_a^2\big)^2]q^2_{a,R_{m+1}}\tilde{\phi}_\sigma$$

and use the representation (2.16) for both terms to the right.

Noting the following generalization of (2.6), cf. Appendix A.2,

$$\|\chi_\nu\mathrm{e}^{\sigma r}|p\phi|\|^2\le 4E\|\chi_\nu\mathrm{e}^{\sigma r}\phi\|^2+C\langle\sigma\rangle^2\|\chi_{\nu/2}\mathrm{e}^{\sigma r}\phi\|^2,\tag{2.22}$$

it follows (for the first term) that

$$\|[\widetilde{H}_a,q^2_{a,R_{m+1}}]\tilde{\phi}_\sigma\|\le C\tfrac{\sigma}{R_{m+1}}\big(\|\tilde{\phi}_\sigma\|+\|\phi\|\big),$$

which agrees with (2.20) provided $R_{m+1}>>R_m$.

We claim that

$$\|[\widetilde{H}_a, \chi^-_{\sigma^2/4}\big(\tilde{p}_a^2\big)^2]q^2_{a,R_{m+1}}\tilde{\phi}_\sigma\| \le C\tfrac{\sigma}{\nu}\big(\|\tilde{\phi}_\sigma\| + \|\phi\|\big), \tag{2.23}$$

which also agrees with (2.20), hence finally showing the latter bound.

Now for showing (2.23) we do various commutation using (2.22)

$$\begin{aligned}
&[\widetilde{H}_a, \chi^-_{\sigma^2/4}\big(\tilde{p}_a^2\big)^2]q^2_{a,R_{m+1}}\tilde{\phi}_\sigma \\
&= O\big(\tfrac{\sigma}{\nu}\big) + [s(x)^{-2}, \chi^-_{\sigma^2/4}\big(\tilde{p}_a^2\big)^2]H^a q^2_{a,R_{m+1}}\tilde{\phi}_\sigma \\
&= O\big(\tfrac{\sigma}{\nu}\big) + O\big(\tfrac{1}{\sigma\nu}\big)\langle\sigma^{-2}\tilde{p}_a^2\rangle^{-1}s(x)^{-1}H^a q^2_{a,R_{m+1}}\phi_\sigma \\
&= O\big(\tfrac{\sigma}{\nu}\big) + O\big(\tfrac{1}{\nu R_{m+1}}\big) + O\big(\tfrac{1}{\sigma\nu}\big)\langle\sigma^{-2}\tilde{p}_a^2\rangle^{-1}s(x)^{-1}q^2_{a,R_{m+1}}H^a\phi_\sigma,
\end{aligned}$$

where we used the convention $\|O\big(\tfrac{\sigma}{\nu}\big)\| \le C\tfrac{\sigma}{\nu}\big(\|\tilde{\phi}_\sigma\| + \|\phi\|\big)$ and similarly for the term $O\big(\tfrac{1}{\nu R_{m+1}}\big)$. Next we decompose

$$\begin{aligned}
H^a\phi_\sigma &= \big((H^\sigma - E + \mathrm{i}\sigma(\operatorname{Re} p^r))\phi_\sigma + \mathrm{i}e^{\sigma(r-4\nu)}R(\nu)\phi\big) \\
&\quad + (E - \mathrm{i}\sigma(\operatorname{Re} p^r) + \tfrac{\sigma^2}{2}|\mathrm{d}r|^2 - \tfrac{1}{2}p_a^2 - I_a)\phi_\sigma - \mathrm{i}e^{\sigma(r-4\nu)}R(\nu)\phi.
\end{aligned}$$

The first term vanishes. The second term contributes with a term of the form $O\big(\tfrac{\sigma}{\nu}\big)$. To see this we use (2.22) in two applications (note that the factor $\langle\sigma^{-2}\tilde{p}_a^2\rangle^{-1}s(x)^{-1}$ is used to bound one factor of p_a^2), and we use the factor $q^2_{a,R_{m+1}}$ (note that $q^2_{a,R_{m+1}}I_a$ is bounded). The third term is $O\big(\tfrac{1}{\nu}\big)$. We have shown (2.23).

3. High-energy hard-core one-body resolvent bound

In Subsections 3.3–3.5 we verify Condition 2.1 for $N = 2$ under Conditions 1.4 and 1.5. The proof will be based on various results for abstract Besov spaces to be given in Subsection 3.1 and on a variant of Mourre theory somewhat related to [Sk3]. We present our main results for the obstacle case in Subsection 3.2. These will be given in a slightly more general setting, and we devote Subsections 3.3 and 3.4 to proofs. The case of an empty obstacle is treated in Subsection 3.5.

3.1. **Abstract Besov spaces.** Let A be a self-adjoint operator on a Hilbert space $\mathcal{H}$. Let $R_0 = 0$ and $R_j = 2^{j-1}$ for $j \in \mathbb{N}$. We define correspondingly characteristic functions $F_j = F(R_{j-1} \le |\cdot| < R_j)$ and the space

$$B = B(A) = \big\{u \in \mathcal{H} \big| \sum_{j\in\mathbb{N}} R_j^{1/2}\|F_j(A)u\| =: \|u\|_B < \infty\big\}. \tag{3.1}$$

We can identify (using the embeddings $\langle A\rangle^{-1}\mathcal{H} \subset B \subset \mathcal{H} \subset B^*$, $\langle A\rangle := \sqrt{A^2+1}$) the dual space B^* as

$$B^* = B(A)^* = \big\{u \in \langle A\rangle\mathcal{H} \big| \sup_{j\ge 1} R_j^{-1/2}\|F_j(A)u\| =: \|u\|_{B^*} < \infty\big\}. \tag{3.2}$$

Alternatively, the elements u of B^* are those sequences $u = (u_j) \subset \mathcal{H}$ with $u_j \in \operatorname{Ran}(F_j(A))$ and $\sup_{j\in\mathbb{N}} R_j^{-1/2}\|u_j\| < \infty$. For previous related works we refer to [AH, JP, GY, Wa, Ro, Sk3] and [Hö, Subsections 14.1 and 30.2]. We note the bounds, cf. [Hö, Subsections 14.1],

$$\|u\|_{B^*} \le \sup_{R>1} R^{-1/2}\|F(|A| < R)u\| \le 2\|u\|_{B^*}. \tag{3.3}$$

Introducing *abstract weighted spaces* $L^2_s = L^2_s(A) = \langle A\rangle^{-s}\mathcal{H}$ we have the embeddings

$$L^2_s \subset B \subset L^2_{1/2} \subset \mathcal{H} \subset L^2_{-1/2} \subset B^* \subset L^2_{-s},\ \text{ for all } s > 1/2. \tag{3.4}$$

All embeddings are continuous and corresponding bounding constants can be chosen as absolute constants, i.e. independently of A and $\mathcal{H}$. In particular

$$\|u\|_{\mathcal{H}} \leq \|u\|_B \text{ for all } u \in B. \tag{3.5}$$

We refer to the spaces B and B^* as *abstract Besov spaces*. Recall the following interpolation type result, here stated abstractly. The proof is the same as that of the concrete versions [AH, Theorem 2.5], [Hö, Theorem 14.1.4], [JP, Proposition 2.3] and [Ro, Subsection 4.3].

Lemma 3.1. *Let A_1 and A_2 be self-adjoint operators on Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$, respectively, and let $s > 1/2$. Suppose $T \in \mathcal{B}(\mathcal{H}_1, \mathcal{H}_2) \cap \mathcal{B}(L^2_s(A_1), L^2_s(A_2))$. Then $T \in \mathcal{B}(B(A_1), B(A_2))$, and there is a constant $C = C(s) > 0$ (independent of T) such that*

$$\|T\|_{\mathcal{B}(B(A_1),B(A_2))} \leq C\big(\|T\|_{\mathcal{B}(\mathcal{H}_1,\mathcal{H}_2)} + \|T\|_{\mathcal{B}(L^2_s(A_1),L^2_s(A_2))}\big). \tag{3.6}$$

We state and prove the following (partial) version of [Sk3, Lemma 2.5].

Lemma 3.2. *Suppose A is a self-adjoint operator on a Hilbert space $\mathcal{H}$, $c > 1$ and $u \in B(A)$, then $u \in B(cA)$ with*

$$\|u\|_{B(cA)} \leq 8c^{1/2}\|u\|_{B(A)}. \tag{3.7}$$

Proof. Pick $i \geq 2$ such that $R_{i-1} < c \leq R_i$. Then for all $j \geq i+1$

$$F_j(ct) \leq F(R_{j-1}/R_i \leq |t| < R_j/R_{i-1}) \leq F_{j-i+1}(t) + F_{j-i+2}(t).$$

Whence for any $u \in B(A)$ we can estimate

$$\begin{aligned}
\|u\|_{B(cA)} &\leq \Big(\sup_{j\geq i+1}\big(R_j/R_{j-i+1}\big)^{1/2} + \sup_{j\geq i+1}\big(R_j/R_{j-i+2}\big)^{1/2}\Big)\|u\|_{B(A)} + \sum_{j=1}^{i} R_j^{1/2}\|u\|_{\mathcal{H}}\\
&\leq \big(2^{(i-1)/2} + 2^{(i-2)/2} + 2^{i/2}(\sqrt{2}+1)\big)\|u\|_{B(A)}\\
&\leq \big(\sqrt{2}+1+2(\sqrt{2}+1)\big)c^{1/2}\|u\|_{B(A)}\\
&\leq 8c^{1/2}\|u\|_{B(A)}.
\end{aligned}$$

□

We note the following abstract version of a result from [JP, Mo2] (proven by using suitable decompositions of unity and the Cauchy Schwarz inequality, see also [Wa, Subsection 2.2]).

Lemma 3.3. *Let A_1 and A_2 be self-adjoint operators on Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$, respectively, and let $T \in \mathcal{B}(\mathcal{H}_1, \mathcal{H}_2)$. Suppose that uniformly in $m, n \in \mathbb{Z}$,*

$$\|F(m \leq A_2 < m+1)TF(n \leq A_1 < n+1)\| \leq C. \tag{3.8}$$

Then with the constant C from (3.8) we have

$$\|T\|_{\mathcal{B}(B(A_1),B(A_2)^*)} \leq 2C. \tag{3.9}$$

We note the following (partial) abstract criterion for (3.8), cf. [Mo2, (I.10)] (see also [Wa]). Recall that a bounded operator T on a Hilbert space is called *accretive* if $T + T^* \geq 0$, cf. for example [RS, Chapter X].

Lemma 3.4. *Let A be a self-adjoint operator on a Hilbert space $\mathcal{H}$, and suppose $T \in \mathcal{B}(\mathcal{H})$ is accretive. Suppose the following bounds uniformly in $n \in \mathbb{Z}$,*

$$\|F(n \le A < n+1)TF(n \le A < n+1)\| \le C_1,$$
$$\|F(A < n)TF(n \le A < n+1)\| \le C_2,$$
$$\|F(n \le A < n+1)TF(A \ge n)\| \le C_3.$$

Then (3.8) *holds with $A_1 = A_2 = A$, the accretive T and with $C = 2C_1 + C_2 + C_3$.*

3.2. **Setting of problem.** Suppose $\Omega \subset \mathbf{X} = \mathbb{R}^d$ is open and $\Theta := \mathbf{X} \setminus \overline{\Omega} \neq \emptyset$ is bounded with smooth boundary $\partial\Theta = \partial\Omega$. Moreover suppose Θ is strictly convex, see Appendix B for definition. The case $\Omega = \mathbf{X}$ is simpler and will be treated in Subsection 3.5.

We consider a Hilbert space $\mathcal{H} = L^2(\Omega, \mathrm{d}x) \otimes L^2(M, \mathrm{d}y)$. The structure of the second factor will not be of importance. To make contact to (2.12) we think of Ω as Ω_b, x as x^b and y as x_b (here $b \notin \{a_{\min}, a_{\max}\}$ and $\#b = N$). Hence the function s of (2.12) is now a function of x and y, viz. $s = s(x, y)$. The operator $\widetilde{H}_b$ takes the form $\widetilde{H}_b = \tilde{H}^b + \tilde{B}_b$ on $\mathcal{H}$. We simplify notation and look at

$$\begin{aligned} H &= \widetilde{H}^b + \widetilde{B}; \\ \widetilde{H}^b &= s(x,y)^{-1}(\tfrac{1}{2}p_x^2 + V(x))s(x,y)^{-1} = \tilde{p}_x^2 + V(x)s(x,y)^{-2}, \\ \widetilde{B} &= \widetilde{B}(x), \end{aligned}$$

where the operator $\widetilde{B}(x)$ acts as a bounded operator on the component $L^2(M, \mathrm{d}y)$. As an operator on $\mathcal{H}$ it is bounded, and it needs to be small and regular in x in a certain sense (to be specified in (3.19c)-(3.19e)). Whence our method does not require much specific structure of the operator-valued potential $\widetilde{B}$. The unbounded part, $\widetilde{H}^b$, is defined with Dirichlet boundary condition at $\partial\Omega$, and the two-body potential $V = V(x)$ needs to be sufficiently regular. For simplicity we impose $V \in C^\infty(\overline{\Omega})$ and $\partial_x^\alpha V(x) = O\big(|x|^{-\varepsilon-|\alpha|}\big)$, cf. Condition 1.4 (1). Whence the form domain of $\widetilde{H}^b$ is given by the space

$$Q(\widetilde{H}^b) = Q(H) = L^2(M, H_0^1(\Omega); \mathrm{d}y) \subset \mathcal{H}.$$

The reader should keep in mind the rough approximation $\widetilde{H}^b \approx -\Delta_x + 2V(x)$ (recall here that $s \approx 1/\sqrt{2}$ in the large ν regime). We denote the resolvent of $H_\sigma := \sigma^{-2}H$ by $R(z, \sigma)$, viz. $R(z, \sigma) = (H_\sigma - z)^{-1}$.

We introduce a function $r = r(x)$ that is different from the function r of Section 2. It is now given as

$$r(x) = \mathrm{dist}(x, \partial\Omega), \tag{3.11a}$$

which can be extended to a smooth function on $\mathbf{X}$ and which at infinity has bounds

$$\partial^\alpha r = O\big(r^{1-|\alpha|}\big) = O\big(\langle x\rangle^{1-|\alpha|}\big). \tag{3.11b}$$

More importantly there exists $c > 0$ such that

$$\nabla^2 r_{|\{r(x)=r\}} \ge \tfrac{c}{1+r} I. \tag{3.11c}$$

The verification of (3.11b) and (3.11c) is given in Appendix B. Note the following consequence of (3.11c),

$$\forall \delta \in (0,1] : \tfrac{\nabla^2 r^2}{2} \geq \delta \mathrm{d}r \otimes \mathrm{d}r \oplus r\nabla^2 r_{|\{r(x)=r\}} \geq \min(\delta, c)\tfrac{r}{1+r} I.$$

In terms of the function r we introduce a conjugate operator different from the operator A that appears in Lemma 1.3. Now

$$A := \tfrac{\nabla r^2}{2} \cdot p + p \cdot \tfrac{\nabla r^2}{2}. \tag{3.12}$$

This operator is self-adjoint on $L^2(\Omega, \mathrm{d}x)$ (it is essentially self-adjoint on $C_c^\infty(\Omega)$) and whence also on $\mathcal{H}$. Note that $Q(H)$ is "boundedly stable" under the dynamics generated by A (using here terminology of [GGM], see also [FMS]), i.e.

$$\forall \psi \in Q(H) : \sup_{|t|<1} \|\mathrm{e}^{\mathrm{i}tA}\psi\|_{Q(H)} < \infty. \tag{3.13a}$$

We note the representation $A = rp_r + p_r r$ where

$$p_r := \tfrac{\nabla r}{2} \cdot p + p \cdot \tfrac{\nabla r}{2} = -\mathrm{i}\tfrac{\partial}{\partial r} - \mathrm{i}\tfrac{\Delta r}{2}.$$

In turn the operator p_r is symmetric as an operator with domain $H_0^1(\Omega)$, and we define p_r^2 as the Friedrichs extension from $C_c^2(\Omega)$ and use the same notation for $p_r^2 \otimes I$. Note the inclusion $Q(H) \subset Q(p_r^2)$ for form domains as well as the following analogue of (3.13a)

$$\forall \psi \in Q(p_r^2) : \sup_{|t|<1} \|\mathrm{e}^{\mathrm{i}tA}\psi\|_{Q(p_r^2)} < \infty. \tag{3.13b}$$

Note for (3.13a) and (3.13b) that a similar property is derived in Appendix A for the conjugate operator used in Section 2 (the one constructed by the Graf vector field). Note for (3.13b) the explicit formula $\|p_r \mathrm{e}^{\mathrm{i}tA}\psi\| = \mathrm{e}^{2t}\|p_r\psi\|$. For a different proof, given in a generalized setting, see Lemma A.11. The property (3.13a) follows from Lemma A.7.

We recall the Hardy bounds, cf. [Da, Lemma 5.3.1],

$$\|r^{-\kappa}|p_r|^{-\kappa}\| \leq 2 \text{ for } \kappa \in [0,1]. \tag{3.14}$$

Moreover we have

$$-\Delta_x = p_r^2 + L^2 + \tfrac{1}{4}(\Delta r)^2 + \tfrac{1}{2}(\partial_r \Delta r), \tag{3.15}$$

where the second term is positive and commutes with r (it is the Laplace-Beltrami operator in geodesic coordinates), and the third and fourth terms are bounded functions on Ω.

We also introduce operators $f_1, f_2 \geq 0$ with squares

$$\begin{aligned} f_1^2 &= \sigma^{-2/3} + \tfrac{r}{1+r}, \\ f_2^2 &= \sigma^{-2/3} + \tfrac{r}{1+r} + \sigma^{-2}p_r^2 = f_1^2 + \sigma^{-2}p_r^2. \end{aligned}$$

A main preliminary bound of this section is

Lemma 3.5. *With A given by* (3.12) *we have uniformly in all large $\sigma, \nu > 1$ and all $\operatorname{Re} z \approx 1$*

$$\|f_2 R(z,\sigma) f_2\|_{\mathcal{B}(B(A),B(A)^*)} \leq C. \tag{3.16}$$

The main result of the section is

Proposition 3.6. *With r given as the multiplication operator on $\mathcal{H}$ in terms of the function* (3.11a) *we have uniformly in all large $\sigma,\nu > 1$ and all* $\operatorname{Re} z \approx 1$

$$\|R(z,\sigma)\|_{\mathcal{B}(B(r),B(r)^*)} \le C\sigma. \tag{3.17}$$

Obviously for b with $\#b = N$ and $\Omega_b \neq \mathbf{X}^b$, and under the regularity conditions on $\Omega = \Omega_b$ and $V_b = V$ introduced above, the bound (2.12) is a consequence of Proposition 3.6.

3.3. **Besov space bound of resolvent, Lemma 3.5.** In this subsection we shall prove Lemma 3.5 using a variant of Mourre theory.

3.3.1. *First order commutator.* We "compute" the commutator

$$\begin{aligned} \mathrm{i}[H,A] &:= s^{-1}\big(2p_r^2 + 2p_i r(\nabla^2 r)^{ij}p_j + W\big)s^{-1} \\ &\quad + 2\mathrm{Re}\,\big(s^{-1}(\nabla r^2\cdot\nabla_x s)\widetilde{H}^b\big) - \nabla r^2\cdot\nabla_x\widetilde{B}; \\ W(x) &:= \tfrac12(\Delta r)^2 + \partial_r\Delta r - \tfrac14\Delta^2 r^2 - \nabla r^2\cdot\nabla V(x). \end{aligned} \tag{3.18}$$

Thus at this stage the first order commutator $\mathrm{i}[H,A]$ is defined by its formal expression. We note that it is a bounded quadratic form on $Q(H)$. The term W is a bounded function, and the second and third terms are "small". More precisely in terms of the parameters ν and σ of Section 2 we have uniform bounds, cf. (1.11c), (2.11) and (2.16),

$$|\tfrac{1+r}{rs}\nabla r^2\cdot\nabla_x s| \le C\nu^{-1}, \tag{3.19a}$$
$$|\tfrac{1+r}{r}(\nabla r^2\cdot\nabla_x)^2 s| \le C, \tag{3.19b}$$
$$\|\tfrac{1+r}{r}\nabla r^2\cdot\nabla_x\widetilde{B}\| \le C\tfrac{\sigma^2}{\nu}, \tag{3.19c}$$
$$\|\tfrac{1+r}{r}(\nabla r^2\cdot\nabla_x)^2\widetilde{B}\| \le C\sigma^2, \tag{3.19d}$$
$$0 \le \widetilde{B} \le \tfrac78\sigma^2. \tag{3.19e}$$

We can estimate the second term after commutation as

$$2\mathrm{Re}\,\big(s^{-1}(\nabla r^2\cdot\nabla_x s)\widetilde{H}^b\big) \ge -C_1\nu^{-1}\big(\mathrm{Re}\,\big(\tfrac{r}{1+r}H\big) + C_2\big),$$

cf. (3.19a) and (3.19e).

Similarly we can estimate the third term as

$$-\nabla r^2\cdot\nabla_x\widetilde{B} \ge -C\tfrac{\sigma^2}{\nu}\tfrac{r}{1+r},$$

cf. (3.19c).

Using these bounds, (3.11c) and (3.14) we can estimate for some small $\delta > 0$ (and uniformly in $\sigma,\nu > 1$)

$$\begin{aligned} \mathrm{i}[\sigma^{-2}H,A] &\ge \sigma^{-2}3p_r^2 + \delta\Big(\sigma^{-2}r^{-2} + \mathrm{Re}\,\big(\tfrac{r}{1+r}\sigma^{-2}\widetilde{H}^b\big)\Big) \\ &\quad - C_1\nu^{-1}\mathrm{Re}\,\big(\tfrac{r}{1+r}\sigma^{-2}H\big) - C_3(\sigma^{-2} + \nu^{-1}\tfrac{r}{1+r}). \end{aligned} \tag{3.20}$$

Next we estimate using (3.19e)

$$\mathrm{Re}\,\big(\tfrac{r}{1+r}\sigma^{-2}\widetilde{H}^b\big) \ge (\mathrm{Re}\,z - \tfrac78)\tfrac{r}{1+r} + \mathrm{Re}\,\big(\tfrac{r}{1+r}(\sigma^{-2}H - z)\big).$$

We are interested in the regime $\mathrm{Re}\, z \approx 1$. Concretely let us assume that $|1 - \mathrm{Re}\, z| \le \frac{1}{9}$ allowing us to estimate uniformly in the spectral parameter: There exists $\delta' \in (0, 3)$ such that for all such z and all large $\sigma, \nu > 1$

$$\delta\Big(\sigma^{-2} r^{-2} + (\mathrm{Re}\, z - \tfrac{7}{8})\tfrac{r}{1+r}\Big) - C_1\nu^{-1}\mathrm{Re}\, z\tfrac{r}{1+r} - C_3(\sigma^{-2} + \nu^{-1}\tfrac{r}{1+r}) \ge \delta' f_1^2.$$

From (3.20) we thus obtain

$$\mathrm{i}[H_\sigma, A] \ge \delta' f_2^2 + (\delta - C_1\nu^{-1})\mathrm{Re}\left(\tfrac{r}{1+r}(H_\sigma - z)\right). \tag{3.21a}$$

Now let us introduce (cf. the method of [Mo1])

$$R_z(\epsilon) = (H_\sigma - \mathrm{i}\epsilon\mathrm{i}[H_\sigma, A] - z)^{-1};\ \epsilon\, \mathrm{Im}\, z > 0,\ |1 - \mathrm{Re}\, z| \le \tfrac{1}{9}.$$

We only need $|\epsilon| \le 1$, and we note that as a form $H_\sigma - \mathrm{i}\epsilon\mathrm{i}[H_\sigma, A]$ is strictly m-sectorial in the terminology of [Ka, RS], cf. the computation (3.18). The associated operator, cf. [RS, Theorem VIII.17], is invertible if we also assume that $|\mathrm{Im}\, z| >> 1$, and hence the inverse is well-defined with adjoint $R_z(\epsilon)^* = R_{\bar z}(-\epsilon)$ under these conditions. However it follows from a connectedness argument and (3.23b) stated below (with $T = f_2$) that $R_z(\epsilon)$ is well-defined without the condition $|\mathrm{Im}\, z| >> 1$. Note also that $\lim_{\epsilon \to 0} R_z(\epsilon) = R(z, \sigma)$.

We obtain from (3.21a) that

$$\mathrm{i}[H_\sigma, A] \ge \tfrac{\delta'}{2} f_2^2 + (\delta - C_1\nu^{-1})\mathrm{Re}\left(\tfrac{r}{1+r}(H_\sigma - \mathrm{i}\epsilon\mathrm{i}[H_\sigma, A] - z)\right). \tag{3.21b}$$

In fact using (3.15) and (3.18) we compute

$$\begin{aligned}
&\mathrm{Re}\left(\tfrac{r}{1+r}\mathrm{i}\epsilon\mathrm{i}[H_\sigma, A]\right)\\
&= \tfrac{\epsilon}{2\sigma^2}\mathrm{i}[\tfrac{r}{1+r}, \mathrm{i}[H, A]]\\
&= \tfrac{\epsilon}{2\sigma^2}\mathrm{i}[\tfrac{r}{1+r}, s^{-1}2p_r^2 s^{-1} + \mathrm{Re}\left(s^{-1}(\nabla r^2 \cdot \nabla_x s)s^{-1}p_r^2 s^{-1}\right)]\\
&= -\tfrac{\epsilon}{\sigma^2}s^{-1}\Big(2\mathrm{Re}\left(p_r(1+r)^{-2}\right) + \mathrm{Re}\left((\nabla r^2 \cdot \nabla_x s)s^{-1}\mathrm{Re}\left(p_r(1+r)^{-2}\right)\right)\Big)s^{-1}\\
&= -\tfrac{\epsilon}{\sigma^2}\mathrm{Re}\left(p_r g\right),
\end{aligned} \tag{3.22}$$

where $g = g(x, y)$ is a uniformly bounded function, and thus indeed

$$-(\delta - C_1\nu^{-1})\mathrm{Re}\left(\tfrac{r}{1+r}\mathrm{i}\epsilon\mathrm{i}[H_\sigma, A]\right) \le C\sigma^{-2/3} f_2^2 \le \tfrac{\delta'}{2} f_2^2.$$

Due to (3.21b) and the second resolvent equation we have the quadratic estimate

$$\|f_2 R_z(\epsilon)T\|^2 \le C_1\left(|\epsilon|^{-1}\|T^* R_z(\epsilon)T\| + \|T^* R_z(\epsilon)^* \tfrac{r}{1+r}T\|\right).$$

Hence if T is an operator obeying

$$\|f_2^{-1}\tfrac{r}{1+r}T\| \le C_2, \tag{3.23a}$$

then

$$\|f_2 R_z(\epsilon)T\|^2 \le C_1\left(|\epsilon|^{-1}\|T^* R_z(\epsilon)T\| + C_2\|T^* R_z(\epsilon)^* f_2\|\right).$$

This leads to

$$\|f_2 R_z(\epsilon)T\|^2 \le C_3|\epsilon|^{-1}\|T^* R_z(\epsilon)T\| + C_4. \tag{3.23b}$$

We have the examples $T = f_2$ and $T = f_2\langle A\rangle^{-1}$ with bounds independent of all large σ and ν. Indeed for all $\psi \in \mathcal{H}$ (or alternatively for all $\psi \in L^2(\Omega, \mathrm{d}x)$ since the operators act on the first tensor factor only)

$$\begin{aligned}\langle f_2^2\rangle_{\frac{r}{1+r}f_2^{-1}\psi} &\leq \|\psi\|^2 + \langle \sigma^{-2}p_r^2\rangle_{\frac{r}{1+r}f_2^{-1}\psi}\\ &\leq \|\psi\|^2 + \|\sigma^{-1}p_r f_2^{-1}\psi\|^2 + C_1\sigma^{-2}\|f_2^{-1}\psi\|^2\\ &\leq C_2\|\psi\|^2,\end{aligned}$$

proving (3.23a) for these examples.

3.3.2. *Technical lemma.* For $B \in \mathcal{B}(Q(p_r^2), \mathcal{H})$ we define

$$\mathrm{ad}_A(B) = [B, A] = \operatorname*{s-lim}_{t\to 0} \mathrm{i}t^{-1}\big(B\mathrm{e}^{-\mathrm{i}tA} - \mathrm{e}^{-\mathrm{i}tA}B\big)_{|Q(p_r^2)\to\mathcal{H}},$$

provided the right hand side exists. Note that we here use (3.13b). In the terminology of [GGM], $B \in C^1(A_{|Q(p_r^2)}, A_{|\mathcal{H}})$ if the right hand side exists. We use this interpretation of the (repeated) commutators in the following lemma (in turn to be used later).

Lemma 3.7. *Uniformly in all $\sigma > 1$*

$$\|\mathrm{ad}_A(f_2)f_2^{-1}\| \leq C, \tag{3.24a}$$

$$\|\mathrm{ad}_A^2(f_2)f_2^{-1}\| \leq C. \tag{3.24b}$$

Proof. Note the representation (valid for any strictly positive operator S)

$$S^{-1/2} = \pi^{-1}\int_0^\infty s^{-1/2}(S+s)^{-1}\mathrm{d}s.$$

With $S = f_2^2$ we thus obtain (for the first term)

$$\begin{aligned}[f_2, A] &= S^{-1/2}[S, A] + [S^{-1/2}, A]S\\ &= S^{-1/2}[S, A] - \pi^{-1}\int_0^\infty s^{-1/2}(S+s)^{-1}[S, A](S+s)^{-1}\mathrm{d}sS,\end{aligned}$$

where

$$[S, A] = \operatorname*{s-lim}_{t\to 0} \mathrm{i}t^{-1}\big(S\mathrm{e}^{-\mathrm{i}tA} - \mathrm{e}^{-\mathrm{i}tA}S\big)_{|Q(p_r^2)\to Q(p_r^2)^*}$$

is computed (up a factor $-\mathrm{i}$) as

$$\mathrm{i}[S, A] = 2\mathrm{Re}\,(\mathrm{i}[S, rp_r]) = 4\sigma^{-2}p_r^2 - 2r(1+r)^{-2} = 4S - 4f_1^2 - 2r(1+r)^{-2}.$$

In particular

$$-CS \leq \mathrm{i}[S, A] \leq CS,$$

which obviously allows us to conclude that

$$B_1 := S^{-1/2}[S, A]S^{-1/2}$$

is bounded. Similarly we introduce

$$B_2 := \int_0^\infty s^{-1/2}(S+s)^{-1}[S, A](S+s)^{-1}\mathrm{d}sS^{1/2},$$

and it remains to show boundedness of B_2: We write with $f := (f_1^2 + \frac{1}{2}r(1+r)^{-2})^{1/2}$

$$\begin{aligned}B_2 &= CI + \mathrm{i}\int_0^\infty s^{-1/2}(S+s)^{-1}4f^2(S+s)^{-1}\mathrm{d}sS^{1/2}\\ &= C(I - f^2S^{-1}) + \mathrm{i}\int_0^\infty s^{-1/2}[(S+s)^{-1}, 4f^2](S+s)^{-1}\mathrm{d}sS^{1/2}\\ &= C(I - fS^{-1}f - f[f, S^{-1}]) - 4\mathrm{i}\int_0^\infty s^{-1/2}(S+s)^{-1}[S, f^2](S+s)^{-2}\mathrm{d}sS^{1/2}\\ &= B - CfS^{-1}[S,f]S^{-1} - 4\mathrm{i}\int_0^\infty s^{-1/2}(S+s)^{-1}[S,f^2](S+s)^{-2}\mathrm{d}sS^{1/2}.\end{aligned}$$

Using the notation $O(1) = O_{\mathcal{B}(\mathcal{H})}(\sigma^0)$ we have

$$\begin{aligned}\mathrm{i}[S,f] &= \tfrac{p_r}{\sigma}O(1)(\sigma f)^{-1} + \text{ h.c.},\\ \mathrm{i}[S,f^2] &= \tfrac{p_r}{\sigma}O(1)\sigma^{-1} + \text{ h.c.} = \sigma^{-2/3}S^{1/2}O(1)S^{1/2},\end{aligned}$$

and the first identity yields that also

$$\begin{aligned}\mathrm{i}fS^{-1}[S,f]S^{-1} &= \big(fS^{-1}\tfrac{p_r}{\sigma}\big)O(1)(\sigma f)^{-1}S^{-1} + fS^{-1}(\sigma^{2/3}f)^{-1}O(1)\big(\sigma^{-1/3}\tfrac{p_r}{\sigma}S^{-1}\big)\\ &= O(1)\sigma^{-2/3}S^{-1} + fS^{-1}\sigma^{-1/3}O(1) = O(1);\end{aligned}$$

i.e. the term is uniformly bounded. The second identity yields that the integral is bounded by

$$\begin{aligned}&C\sigma^{-2/3}\int_0^\infty s^{-1/2}\|(S+s)^{-1}S^{1/2}(S+s)^{-1}\|\mathrm{d}s\\ &\le C\sigma^{-2/3}\int_0^\infty s^{-1/2}(\sigma^{-2/3}+s)^{-3/2}\mathrm{d}s,\end{aligned} \tag{3.25}$$

and since the latter integral is independent of σ indeed also the integral is uniformly bounded. So also B_2 is uniformly bounded and (3.24a) follows.

As for (3.24b) we use a previous computation to obtain

$$\begin{aligned}-\mathrm{ad}_A^2(S) &= 4\big(4S - 4f_1^2 - 2r(1+r)^{-2}\big) + 2r\tfrac{\partial}{\partial r}\big(4f_1^2 + 2r(1+r)^{-2}\big)\\ &= 16S - 16\tilde{f}^2;\ \tilde{f} = \Big(\sigma^{-2/3} + \frac{\frac{3}{4}r + \frac{9}{4}r^2 + r^3}{(1+r)^3}\Big)^{1/2}.\end{aligned}$$

which leads to form-boundedness

$$\|S^{-1/2}\mathrm{ad}_A^2(S)S^{-1/2}\| \le C.$$

We decompose

$$\begin{aligned}&\mathrm{ad}_A^2(f_2)S^{-1/2} = T_1 + \cdots + T_5;\\ &T_1 = \mathrm{ad}_A(S^{-1/2})\,\mathrm{ad}_A(S)S^{-1/2} = \big(\mathrm{ad}_A(S^{-1/2})S^{1/2}\big)\big(S^{-1/2}\mathrm{ad}_A(S)S^{-1/2}\big),\\ &T_2 = S^{-1/2}\mathrm{ad}_A^2(S)S^{-1/2},\\ &T_3 = -\pi^{-1}\int_0^\infty s^{-1/2}(S+s)^{-1}\mathrm{ad}_A^2(S)(S+s)^{-1}\mathrm{d}sS^{1/2},\\ &T_4 = \pi^{-1}\int_0^\infty s^{-1/2}(S+s)^{-1}\mathrm{ad}_A(S)(S+s)^{-1}\mathrm{ad}_A(S)(S+s)^{-1}\mathrm{d}sS^{1/2},\\ &T_5 = -\pi^{-1}\int_0^\infty s^{-1/2}(S+s)^{-1}\mathrm{ad}_A(S)(S+s)^{-1}\mathrm{ad}_A(S)(S+s)^{-1}s\mathrm{d}sS^{-1/2}.\end{aligned}$$

The boundedness of the term T_1 follows from the previous proof. Clearly the term T_2 is bounded. We can show boundedness of T_3 as we proceeded for (3.24a) (note that now $\tilde f$ plays the role of the previous f). For T_4 and T_5 we rewrite

$$\begin{aligned} &T_4 + T_5 = \widetilde{T}_4 + \widetilde{T}_5;\\ &\quad \widetilde{T}_4 = \pi^{-1}\int_0^\infty s^{-1/2}(S+s)^{-1}\mathrm{ad}_A(S)(S+s)^{-1}\mathrm{d}s\, S^{1/2}\big(S^{-1/2}\mathrm{ad}_A(S)S^{-1/2}\big),\\ &\quad \widetilde{T}_5 = -2\pi^{-1}\int_0^\infty s^{-1/2}(S+s)^{-1}\mathrm{ad}_A(S)(S+s)^{-1}\mathrm{ad}_A(S)(S+s)^{-1}s\mathrm{d}sS^{-1/2}. \end{aligned}$$

The boundedness of the term $\widetilde{T}_4$ follows from the previous proof. Whence it only remains to show boundedness of $\widetilde{T}_5$. We proceed in a similar fashion as before substituting for the first factor of $\mathrm{ad}_A(S)$ from the left $\mathrm{ad}_A(S) = -\mathrm{i}4(S - f^2)$ and then move to the left. The commutator is treated as in (3.25) using now also the form-boundedness of the second factor of $\mathrm{ad}_A(S)$. So it remains to consider

$$(I - f^2S^{-1})\int_0^\infty s^{-1/2}S(S+s)^{-2}\mathrm{ad}_A(S)(S+s)^{-1}S^{-1/2}s\mathrm{d}s.$$

We saw before that the first factor is bounded. For the integral we substitute again $\mathrm{ad}_A(S) = -\mathrm{i}4(S - f^2)$ and move to the left. Estimating as in (3.25) we conclude that the commutator is bounded. So we are left with

$$\int_0^\infty \cdots \mathrm{d}s = C_1(S - f^2)\int_0^\infty s^{-1/2}S(S+s)^{-3}S^{-1/2}s\mathrm{d}s = C_2(I - f^2S^{-1}),$$

which is bounded. Whence (3.24b) follows. □

3.3.3. *Second order commutator.* In (3.18) we took the formal commutator as a definition of $\mathrm{i}[H,A]$, however due to the property (3.13a) there is the following alternative interpretation

$$-\mathrm{i}[H,A] = \operatorname*{s-lim}_{t\to 0} t^{-1}\big(H\mathrm{e}^{-\mathrm{i}tA} - \mathrm{e}^{-\mathrm{i}tA}H\big)_{|Q(H)\to Q(H)^*}, \tag{3.26}$$

cf. Lemma A.9 and [GGM], which allows us to compute

$$\frac{\mathrm{d}}{\mathrm{d}\epsilon}R_z(\epsilon) = -R_z(\epsilon)[H_\sigma, A]R_z(\epsilon) = R_z(\epsilon)A - AR_z(\epsilon) + \epsilon R_z(\epsilon)\mathrm{ad}_A^2(H_\sigma)R_z(\epsilon), \tag{3.27}$$

where $\mathrm{ad}_A^2(H_\sigma) = [[H_\sigma, A], A] \in \mathcal{B}(Q(H), Q(H)^*)$. Note that in the terminology of [GGM], $H \in C^2(A_{|Q(H)}, A_{|Q(H)^*})$. The second identity of (3.27) is valid as a form on the domain $\mathcal{D}^* := \mathcal{D}\big(A_{|Q(H)^*}\big)$ of the generator of the extended group $\{\mathrm{e}^{-\mathrm{i}tA}\}_{|Q(H)^*}$, so that indeed $A : \mathcal{D}^* \to Q(H)^*$, which combines with the mapping property $R_z(\epsilon) : Q(H)^* \to Q(H)$. Below we use tacitly this interpretation and the fact that $f_2\langle A\rangle^{-1} : \mathcal{H} \to \mathcal{D}^*$, cf. (3.24a).

Using (3.14) (with $\kappa = 1/2$), (3.18) and (3.19a)-(3.19d) we compute

$$\mathrm{ad}_A^2(H_\sigma) = f_2B_0f_2 + \sum_{i,j=1}^{\dim \mathbf{X}} \big(\tfrac{r}{1+r}\big)^{1/2}(\sigma s)^{-1}p_iB_{ij}p_j(\sigma s)^{-1}\big(\tfrac{r}{1+r}\big)^{1/2}, \tag{3.28}$$

where p_j denotes the components of p_x and all B's are uniformly bounded.

Using (3.23b), (3.27) and (3.28) we shall prove three bounds which are uniform in z and ϵ as specified above and (for convenience) with $\mathrm{Im}\, z, \epsilon > 0$ as well as uniform in (large) σ and ν:

$$\|F_z(\epsilon)\| \leq C \text{ for } F_z(\epsilon) := \langle A\rangle^{-1} f_2 R_z(\epsilon) f_2 \langle A\rangle^{-1}, \tag{3.29a}$$

$$\|F_z^-(\epsilon)\| \leq C \text{ for } F_z^-(\epsilon) := \mathrm{e}^{\epsilon A} F(A<0) f_2 R_z(\epsilon) f_2 \langle A\rangle^{-2}, \tag{3.29b}$$

$$\|F_z^+(\epsilon)\| \leq C \text{ for } F_z^+(\epsilon) := \langle A\rangle^{-2} f_2 R_z(\epsilon) f_2 F(A\geq 0)\mathrm{e}^{-\epsilon A}. \tag{3.29c}$$

Re (3.29a)**.** Due to (3.23b) for $T = f_2\langle A\rangle^{-1}$ (note that we proved (3.23a))

$$\|F_z(\epsilon)\| \leq C\epsilon^{-1} \text{ for } 0 < \epsilon \leq 1. \tag{3.30}$$

Obviously (3.24a) yields the bounds

$$\|f_2^{-1} A f_2 \langle A\rangle^{-1}\| \leq C \text{ and } \|\langle A\rangle^{-1} f_2 A f_2^{-1}\| \leq C. \tag{3.31}$$

Exploiting (3.23b), (3.27), (3.28) and (3.31) we can show that

$$\Big\|\frac{\mathrm{d}}{\mathrm{d}\epsilon} F_z(\epsilon)\Big\| \leq C\big(\epsilon^{-1/2}\|F_z(\epsilon)\|^{1/2} + \|F_z(\epsilon)\| + \widetilde{C}\big). \tag{3.32}$$

Here we can argue as follows for the contribution to (3.27) from the second term in (3.28). For $\psi \in \mathcal{H}$ we estimate using (3.14), (3.19e) and (3.22)

$$\begin{aligned} \sum_j \|p_j(\sigma s)^{-1}\big(\tfrac{r}{1+r}\big)^{1/2}\psi\|^2 &\leq C_1\|f_2\psi\|^2 + 2\mathrm{Re}\,\langle H_\sigma - z\rangle_{r^{1/2}(1+r)^{-1/2}\psi} \\ &\leq C_2\|f_2\psi\|^2 + 2\mathrm{Re}\,\langle \tfrac{r}{1+r}(H_\sigma - \mathrm{i}\epsilon\mathrm{i}[H_\sigma, A] - z\rangle_\psi. \end{aligned} \tag{3.33a}$$

We use (3.33a) to $\psi = R_z(\epsilon) f_2\langle A\rangle^{-1}\tilde{\psi}$, $\tilde{\psi}\in\mathcal{H}$, and then (3.23a) and (3.23b) with $T = f_2\langle A\rangle^{-1}$. Similarly we apply

$$\sum_i \|p_i(\sigma s)^{-1}\big(\tfrac{r}{1+r}\big)^{1/2}\psi\|^2 \leq C_2\|f_2\psi\|^2 + 2\mathrm{Re}\,\langle \tfrac{r}{1+r}(H_\sigma + \mathrm{i}\epsilon\mathrm{i}[H_\sigma, A] - \bar{z}\rangle_\psi \tag{3.33b}$$

to $\psi = R_{\bar z}(-\epsilon) f_2\langle A\rangle^{-1}\tilde{\psi}$. We conclude (3.32).

Clearly (3.29a) follows from (3.30) and (3.32) by two integrations.

Re (3.29b)**.** Due to (3.23b) and (3.29a)

$$\|F_z^-(\epsilon)\| \leq C\epsilon^{-1/2}. \tag{3.34}$$

Using (3.27) we compute

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}\epsilon} F_z^-(\epsilon) &= T_1 + T_2 + T_3; \\ T_1 &= \mathrm{e}^{\epsilon A} F(A<0)[A, f_2] R_z(\epsilon) f_2\langle A\rangle^{-2}, \\ T_2 &= \mathrm{e}^{\epsilon A} F(A<0) f_2 R_z(\epsilon) A f_2 \langle A\rangle^{-2}, \\ T_3 &= \epsilon\mathrm{e}^{\epsilon A} F(A<0) f_2 R_z(\epsilon)\mathrm{ad}_A^2(H_\sigma) R_z(\epsilon) f_2\langle A\rangle^{-2}. \end{aligned} \tag{3.35}$$

Using again (3.23b) and (3.29a) we can estimate

$$\|T_j\| \leq C\epsilon^{-1/2} \text{ for } 0<\epsilon\leq 1 \text{ and } j = 1,2,3. \tag{3.36}$$

Notice that for all of the terms T_1–T_3 we apply (3.23b) with $T = f_2\langle A\rangle^{-1}$, Lemma 3.7 and in addition for T_3 we apply (3.23b) with $T = f_2$ and (3.33a)–(3.33b). Clearly (3.29b) follows from (3.34)–(3.36) by one integration.

Re (3.29c)**.** We mimic the proof of (3.29b).

Next we note that the above arguments apply to $A \to A-n$ for any $n \in \mathbb{Z}$ yielding bounds being independent of n. Taking $\epsilon \to 0$ we thus obtain the following bounds for the accretive operator $T(z) = -\mathrm{i}f_2R(z,\sigma)f_2$, all being uniform in n and in large σ and ν,

$$\|\langle A-n\rangle^{-1}T(z)\langle A-n\rangle^{-1}\| \leq \tilde{C},$$
$$\|F(A<n)T(z)\langle A-n\rangle^{-2}\| \leq \tilde{C},$$
$$\|\langle A-n\rangle^{-2}T(z)F(A\geq n)\| \leq \tilde{C}.$$

Due to these bounds and Lemmas 3.3–3.4 we conclude (3.16) with $C = 16\tilde{C}$ provided $\operatorname{Im} z > 0$ (and hence also if $\operatorname{Im} z < 0$).

3.4. **Besov space bound of resolvent, Proposition 3.6.** We introduce operators

$$S_\sigma = f_2^{-1}f_1 \text{ and } T_\sigma = M(t_\sigma);\ t_\sigma(r) = \sigma\big(\tfrac{r}{1+r}\big)^{1/2}(1+r)f_1^2.$$

Here and henceforth $M(\cdot)$ refers to the operator of multiplication by the function in the argument. We shall prove the following lemmas

Lemma 3.8. *There exists $C>0$ independent of $\sigma>1$ such that*

$$\|S_\sigma v\|_{B(A)} \leq C\|v\|_{B(T_\sigma)}. \tag{3.38}$$

Lemma 3.9. *There exists $C>0$ independent of $\sigma>1$ such that*

$$\|f_1^{-1}u\|_{B(T_\sigma)} \leq C\sigma^{1/2}\|u\|_{B(r)}. \tag{3.39}$$

Proof of Proposition 3.6. We combine Lemmas 3.8–3.9 to obtain that

$$f_2^{-1} = S_\sigma f_1^{-1} \in \mathcal{B}(B(r), B(A))$$

with a bounding constant of the form $C\sigma^{1/2}$. Whence, due to Lemma 3.5,

$$R(z,\sigma) = f_2^{-1}\big(f_2R(z,\sigma)f_2\big)f_2^{-1} \in \mathcal{B}(B(r), B(r)^*)$$

with a bounding constant of the form $C\sigma$. □

Proof of Lemma 3.8. Since $\|S_\sigma\| \leq 1$ it suffices, due to Lemma 3.1, to show the bound

$$\|AS_\sigma v\| \leq C\big(\|T_\sigma v\| + \|v\|\big). \tag{3.40}$$

Using (3.24a) we estimate for all $\psi \in \mathcal{D}(r) = \mathcal{D}(M(r))$

$$\begin{aligned}\|Af_2^{-1}\psi\|^2 &\leq 2\|f_2^{-1}A\psi\|^2 + C_1\|f_2^{-1}\psi\|^2\\ &\leq 4\|f_2^{-1}2p_r r\psi\|^2 + C_2\|f_2^{-1}\psi\|^2\\ &\leq 16\sigma^2\|r\psi\|^2 + C_2\|S_\sigma f_1^{-1}\psi\|^2\\ &\leq 16\sigma^2\|\big(\tfrac{r}{1+r}\big)^{1/2}(1+r)f_1\psi\|^2 + C_2\|f_1^{-1}\psi\|^2.\end{aligned}$$

We apply the estimate to $\psi = f_1 v$ yielding (3.40) with $C = \max(4, C_2^{1/2})$. □

Proof of Lemma 3.9. Introducing $\tilde f_1 = \sigma^{1/2} f_1$ we need to bound for $j = 1, 2, 3$

$$\|\tilde f_1^{-1} F_j u\|_{B(T_\sigma)} \leq C\|u\|_{B(r)}; \tag{3.41}$$
$$F_1 = F(r < \sigma^{-2/3}),$$
$$F_2 = F(\sigma^{-2/3} \leq r < 2),$$
$$F_2 = F(r \geq 2).$$

Using that t_σ is a bounded function on the support of F_1 and (3.5) we estimate

$$\|\tilde f_1^{-1} F_1 u\|_{B(T_\sigma)} \leq C_1 \sigma^{-1/6}\|u\| \leq C_1\|u\|_{B(r)}, \tag{3.42a}$$

which agrees with (3.41).

Let $g_\sigma(r) = \sigma r^{3/2}$ and $G_\sigma = M(g_\sigma)$. Using the two-sided estimates $t_\sigma(r) \leq C g_\sigma(r)$ and $g_\sigma(r) \leq C t_\sigma(r)$, which are valid on the support of F_2, we can estimate

$$\begin{aligned}\|\tilde f_1^{-1} F_2 u\|_{B(T_\sigma)} &\leq C\|\big(\sigma r\big)^{-1/2} F_2 u\|_{B(G_\sigma)}\\ &= C \sum_{2\leq j\leq J} R_j^{1/2}\|F(R_{j-1} \leq g_\sigma(r) < R_j)(\sigma r^{3/2})^{-1/2} r^{1/4} F_2 u\|\\ &\leq 2^{1/2} C \sum_{2\leq j\leq J} \|F(R_{j-1} \leq g_\sigma(r) < R_j) r^{1/4} F_2 u\|,\end{aligned}$$

where $J = J_\sigma \in \mathbb{N}$ is taken smallest such that $R_J > 2^{3/2}\sigma$. By estimating for each term

$$r^{1/4} \leq \big(R_j/\sigma\big)^{1/6} \leq 2^{(j-J+3)/6},$$

we thus obtain

$$\|\tilde f_1^{-1} F_2 u\|_{B(T_\sigma)} \leq 2^{1/2} C \sum_{2\leq j\leq J} 2^{(j-J+3)/6}\|u\| \leq C_1\|u\|_{B(r)}, \tag{3.42b}$$

which also agrees with (3.41).

Finally using the two-sided estimates $t_\sigma(r) \leq C\sigma(1+r)$ and $\sigma(1+r) \leq C t_\sigma(r)$, which are valid on the support of F_3, and Lemma 3.2 we can estimate

$$\begin{aligned}\|\tilde f_1^{-1} F_3 u\|_{B(T_\sigma)} &\leq C_1 \sigma^{-1/2}\|u\|_{B(\sigma(1+r))}\\ &\leq 8C_1\|u\|_{B((1+r))} \leq C_2\|u\|_{B(r)},\end{aligned} \tag{3.42c}$$

which also agrees with (3.41).

Having proved (3.42a)–(3.42c) we conclude (3.41). □

3.5. **Case $\Omega = \mathbf{X}$.** We outline a proof of the analogue of Proposition 3.6 for the case $\Omega = \mathbf{X}$. This is conceptionally simpler than the previous case, and it suffices to mimic parts of the previous proof. We can use the standard conjugate operator

$$A = x \cdot p + p \cdot x, \tag{3.43}$$

rather than the one defined by (3.12) (alternatively A is given by taking $r = |x|$ in (3.12)). We impose

$$V(x), x\cdot\nabla V(x), \, (x\cdot\nabla)^2 V(x) \in \mathcal{C}\big(H^1(\mathbf{X}), H^1(\mathbf{X})^*\big). \tag{3.44}$$

We consider a Hilbert space $\mathcal{H} = L^2(\mathbf{X}, \mathrm{d}x) \otimes L^2(M, \mathrm{d}y)$ where interpretation of x, y and M is the same as in Subsection 3.2. Similarly introducing $H = \widetilde{H}^b + \widetilde{B}$ as before the form domains are

$$Q(\widetilde{H}^b) = Q(H) = L^2(M, H^1(\mathbf{X}); \mathrm{d}y) \subset \mathcal{H}.$$

Again we have the property (3.13a). We define

$$f^2 = 1 + \sigma^{-2}p^2, f \geq 0.$$

We have results similar to Lemma 3.5 and Proposition 3.6.

Lemma 3.10. *With A given by* (3.43) *we have uniformly in all large $\sigma, \nu > 1$ and all $\operatorname{Re} z \approx 1$*

$$\|fR(z, \sigma)f\|_{\mathcal{B}(B(A),B(A)^*)} \leq C. \tag{3.45}$$

Proposition 3.11. *We have uniformly in all large $\sigma, \nu > 1$ and all $\operatorname{Re} z \approx 1$*

$$\|R(z, \sigma)\|_{\mathcal{B}(B(|x|),B(|x|)^*)} \leq C\sigma. \tag{3.46}$$

Given Lemma 3.10 we notice that Proposition 3.11 is an easy consequence of the following analogues of Lemmas 3.8 and 3.9. Define

$$T_\sigma = M(t_\sigma);\ t_\sigma(x, y) = \sigma(1 + |x|).$$

Lemma 3.12. *There exists $C > 0$ independent of $\sigma > 1$ such that*

$$\|f^{-1}v\|_{B(A)} \leq C\|v\|_{B(T_\sigma)}. \tag{3.47}$$

Lemma 3.13. *There exists $C > 0$ independent of $\sigma > 1$ such that*

$$\|u\|_{B(T_\sigma)} \leq C\sigma^{1/2}\|u\|_{B(|x|)}. \tag{3.48}$$

We can prove Lemma 3.12 by mimicking the proof of Lemma 3.8, while Lemma 3.13 is an immediate consequence of Lemma 3.2.

Whence it remains to show Lemma 3.10. For that we note the analogue of (3.18) where now $r = |x|$

$$\begin{aligned} \mathrm{i}[H, A] &:= s^{-1}\big(2p^2 + W\big)s^{-1} + 2\mathrm{Re}\,\big(s^{-1}(\nabla r^2 \cdot \nabla_x s)\widetilde{H}^b\big) - \nabla r^2 \cdot \nabla_x \widetilde{B}; \\ W(x) &:= -\nabla r^2 \cdot \nabla V(x). \end{aligned} \tag{3.49}$$

Using (3.49) we can indeed mimic the proof of Lemma 3.5 with f replacing f_2. Note this is much simpler now. For example there are no factors of $\frac{r}{1+r}$ to consider, and the analogue of the second order commutator is given by (3.28) without the second term on the right hand side. We leave the details to the reader.

Appendix A

In this appendix we show how to undo the commutator $\mathrm{i}[H, A]$. This is used to obtain (2.4). Since the Schrödinger operator H is realized with the Dirichlet boundary condition the approximation procedure of [IS2] is not sufficient. We also show (3.13a) and (3.26).

A.1. **Setting.** We shall work in a generalized setting on a manifold, and present all conditions needed for the argument independently of the previous sections. The case of a constant metric is sufficient for application to (2.4). The verification of the conditions below under the conditions of Sections 1 and 2 is straightforward.

Let (Ω, g) be a Riemannian manifold of dimension $d \geq 1$, and consider the Schrödinger operator on $\mathcal{H} = L^2(\Omega) = L^2(\Omega, (\det g)^{1/2}\mathrm{d}x)$:

$$H = H_0 + V; \quad H_0 = -\tfrac{1}{2}\Delta = \tfrac{1}{2}p_i^* g^{ij} p_j, \quad p_i = -\mathrm{i}\partial_i.$$

We realize H_0 as a self-adjoint operator by imposing the Dirichlet boundary condition, i.e. H_0 is the unique self-adjoint operator associated with the closure of the quadratic form

$$\langle H_0 \rangle_\psi = \langle \psi, -\tfrac{1}{2}\Delta\psi \rangle, \quad \psi \in C_{\mathrm{c}}^\infty(\Omega).$$

We denote the form closure and the self-adjoint realization by the same symbol H_0. Moreover, we consider the weighted spaces

$$\mathcal{H}^s = (H_0 + 1)^{-s/2}\mathcal{H}, \quad s \in \mathbb{R},$$

and H_0 may also be understood as $\mathcal{H}^s \to \mathcal{H}^{s-2}$, $s \in \mathbb{R}$. For the realization of $H = H_0 + V$ we assume the following condition:

Condition A.1. The potential V is a locally integrable real-valued function, and there exist $\varepsilon \in [0, 1)$ and $C > 0$ such that for any $\psi \in C_{\mathrm{c}}^\infty(\Omega)$

$$|\langle V \rangle_\psi| \leq \varepsilon \langle H_0 \rangle_\psi + C\|\psi\|^2.$$

By this condition we extend the form domain of V as $Q(V) = \mathcal{H}^1$, and this defines a bounded operator $V \colon \mathcal{H}^1 \to \mathcal{H}^{-1}$. We note, though, this quadratic form is not necessarily closed. We henceforth consider $H = H_0 + V$ as a closed quadratic form on $Q(H) = \mathcal{H}^1$ or, equivalently, as a bounded operator $\mathcal{H}^1 \to \mathcal{H}^{-1}$. Then the Friedrichs self-adjoint realization of H on $\mathcal{H}$ is the restriction of this $H \colon \mathcal{H}^1 \to \mathcal{H}^{-1}$ to the domain:

$$\mathcal{D}(H) = \{\psi \in \mathcal{H}^1 \,|\, H\psi \in \mathcal{H}\} \subset \mathcal{H}.$$

We next assume a regularity condition for the (virtual) boundary of Ω:

Condition A.2. There exists a real-valued function $r \in C^\infty(\Omega)$ such that:

(1) The gradient vector field $2\omega = \operatorname{grad} r^2$ on Ω is complete.
(2) The following bounds hold:

$$\sup|\mathrm{d}r| < \infty, \quad \sup|\nabla^2 r^2| < \infty, \quad \sup|\mathrm{d}\Delta r^2| < \infty. \tag{A.1}$$

The function r of Condition A.2 is a generalization of that of previous sections. For the r of Sections 1 and 2, defined in Subsection 1.3, we refer to Lemma 1.2 for properties. Note that the vector field 2ω is defined and complete on $\mathbf{X} \supset \Omega$ due to Lemma 1.2 (5). The completeness on Ω is then valid intuitively because the vector field is tangent to the boundary $\partial\Omega$, cf. Lemma 1.2 (2). Indeed one can use Lemma 1.2 (2) to show Condition A.2 (1). Similarly Condition A.2 (2) follows from Lemma 1.2 (5). For the r of Subsection 3.2 we refer to (3.11b) (the completeness is valid because 2ω vanishes at the boundary $\partial\Omega \times M$). For the r of Subsection 3.5 the properties (1) and (2) are obvious, however there is a cusp singularity at $x = 0$ in this case. A substitute for Lemmas A.7–A.9, shown under Conditions A.1–A.2, is in this case immediately provided by the formula $\|p\mathrm{e}^{\mathrm{i}tA}\psi\| = \mathrm{e}^{2t}\|p\psi\|$.

By Condition A.2 (1) the vector field 2ω generates a one-parameter group of diffeomorphisms on Ω, which we denote by

$$\mathrm{e}^{2\cdot}\cdot\colon \mathbb{R}\times\Omega\to\Omega,\quad (t,x)\mapsto \mathrm{e}^{2t}x. \tag{A.2}$$

This satisfies by definition, in local coordinates,

$$\partial_t(\mathrm{e}^{2t}x)^i = g^{ij}(\mathrm{e}^{2t}x)(\partial_j r^2)(\mathrm{e}^{2t}x). \tag{A.3}$$

We define the group of *dilations* $\mathrm{e}^{\mathrm{i}tA}\colon \mathcal{H}\to\mathcal{H}$ with respect to r as the one-parameter group of unitary operators

$$\mathrm{e}^{\mathrm{i}tA}u(x) = J(\mathrm{e}^{2t};x)^{1/2}\left(\frac{\det g(\mathrm{e}^{2t}x)}{\det g(x)}\right)^{1/4} u(\mathrm{e}^{2t}x),$$

where J is the relevant Jacobian. Note that there is another expression:

$$\mathrm{e}^{\mathrm{i}tA}u(x) = \exp\left(\int_0^t \tfrac{1}{2}(\Delta r^2)(\mathrm{e}^{2s}x)\,\mathrm{d}s\right) u(\mathrm{e}^{2t}x). \tag{A.4}$$

We let A be the generator of $\mathrm{e}^{\mathrm{i}tA}$. By the unitarity of $\mathrm{e}^{\mathrm{i}tA}$ the operator A is self-adjoint, and $C^\infty_{\mathrm{c}}(\Omega)\subseteq\mathcal{D}(A)$ is a core for it. In fact, the dense subspace $C^\infty_{\mathrm{c}}(\Omega)\subseteq\mathcal{H}$ is invariant under $\mathrm{e}^{\mathrm{i}tA}$, and for any $u\in C^\infty_{\mathrm{c}}(\Omega)$ the limit

$$\lim_{t\to 0} t^{-1}(\mathrm{e}^{\mathrm{i}tA}u-u)$$

exists in $\mathcal{H}$. Note that by (A.4) when applied to vectors in $C^\infty_{\mathrm{c}}(\Omega)$ the operator A takes the form

$$A = \mathrm{i}[H_0,r^2] = \tfrac{1}{2}\{(\partial_i r^2)g^{ij}p_j + p_i^* g^{ij}(\partial_j r^2)\} = rp^r + (p^r)^* r,$$

where $p^r = -\mathrm{i}\partial^r = -\mathrm{i}(\partial_i r)g^{ij}\partial_j$.

Let us first consider the commutator $\mathrm{i}[H,A]$ as a quadratic form defined for $\psi\in C^\infty_{\mathrm{c}}(\Omega)$ by

$$\langle \mathrm{i}[H,A]\rangle_\psi = \mathrm{i}\langle H\psi, A\psi\rangle - \mathrm{i}\langle A\psi, H\psi\rangle.$$

In order to discuss its extension we impose the following abstract form bound condition, which is not quite independent of Conditions A.1 and A.2 (see for example [IS1, Corollary 4.2]).

Condition A.3. There exists $C>0$ such that for any $\psi\in C^\infty_{\mathrm{c}}(\Omega)$

$$|\langle \mathrm{i}[H,A]\rangle_\psi| \le C\langle H_0+1\rangle_\psi.$$

Similarly to the above, we henceforth regard $\mathrm{i}[H,A]$ as a quadratic form on $Q(\mathrm{i}[H,A])=\mathcal{H}^1$ (which may not be closed) or as a bounded operator $\mathcal{H}^1\to\mathcal{H}^{-1}$.

A.2. **Preliminaries.** We prove a regularity property of the flow (A.2).

Lemma A.4. *There exists $C>0$ such that for any $t\in\mathbb{R}$ and $x\in\Omega$*

$$d\mathrm{e}^{-C|t|} \le g^{ij}(x)g_{kl}(\mathrm{e}^{2t}x)[\partial_i(\mathrm{e}^{2t}x)^k][\partial_j(\mathrm{e}^{2t}x)^l] \le d\mathrm{e}^{C|t|}. \tag{A.5}$$

Proof. The proof is similar to that of [IS1, Lemma 2.3]. We note that the expression in the middle of (A.5) is independent of choice of coordinates. Fix $x\in\Omega$ and choose coordinates such that $g_{ij}(x)=\delta_{ij}$. Consider the vector fields along $\{\mathrm{e}^{2t}x\}_{t\in\mathbb{R}}$ given by $\partial_i e^{2t}x$ and $\partial_j e^{2t}x$. Since the Levi-Civita connection ∇ is compatible with the metric,

$$\begin{aligned}\tfrac{\partial}{\partial t} g_{kl}(e^{2t}x)[\partial_i(e^{2t}x)^k][\partial_j(e^{2t}x)^l] &= \tfrac{\partial}{\partial t}\langle \partial_i e^{2t}x, \partial_j e^{2t}x\rangle \\ &= \langle \nabla_{\partial_t e^{2t}x}\partial_i e^{2t}x, \partial_j e^{2t}x\rangle + \langle \partial_i e^{2t}x, \nabla_{\partial_t e^{2t}x}\partial_j e^{2t}x\rangle.\end{aligned} \tag{A.6}$$

(The definition of $\nabla_{\partial_t e^{2t}x}$ is given below.) From (A.3) it follows that

$$\begin{aligned}\nabla_{\partial_t e^{2t}x}\partial_i(e^{2t}x)^\bullet &= \partial_t\partial_i(e^{2t}x)^\bullet + [\partial_t(e^{2t}x)^k]\Gamma^\bullet_{kl}\partial_i(e^{2t}x)^l \\ &= \partial_i\partial_t(e^{2t}x)^\bullet + (g^{km}\partial_m r^2)\Gamma^\bullet_{kl}\partial_i(e^{2t}x)^l \\ &= [\partial_i(e^{2t}x)^k]\partial_k(g^{\bullet l}\partial_l r^2) + [\partial_i(e^{2t}x)^l]\Gamma^\bullet_{kl}g^{km}\partial_m r^2 \\ &= \nabla_{\partial_i e^{2t}x}(g^{\bullet l}\partial_l r^2) \\ &= g^{\bullet l}[\partial_i(e^{2t}x)^k](\nabla^2 r^2)_{kl}.\end{aligned}$$

Thus, plugging this into (A.6) and taking a contraction with $g^{ij}(x) = \delta^{ij}$, we obtain

$$\left|\tfrac{\partial}{\partial t} g^{ij}(x)g_{kl}(e^{2t}x)[\partial_i(e^{2t}x)^k][\partial_j(e^{2t}x)^l]\right| \le Cg^{ij}(x)g_{kl}(e^{2t}x)[\partial_i(e^{2t}x)^k][\partial_j(e^{2t}x)^l].$$

Noting $g^{ij}(x)g_{kl}(e^{2t}x)[\partial_i(e^{2t}x)^k][\partial_j(e^{2t}x)^l]\big|_{t=0} = d$, we have (A.5). □

Recall the functions $\chi_\nu, \bar\chi_\nu \in C^\infty(\mathbb{R})$ of Subsubsection 1.3.3. We shall henceforth consider the functions $\chi_\nu = \chi_\nu(r)$, $\bar\chi_\nu = \bar\chi_\nu(r)$ as being composed with the function r from Condition A.2. We also set

$$\chi_{\nu,\nu'} = \chi_\nu\bar\chi_{\nu'}, \quad \bar\chi_{\nu'} = 1 - \chi_{\nu'}, \quad \nu' \ge 2\nu \ge 2.$$

Next, we prove the following statement:

Lemma A.5. *Let $\psi \in \mathcal{D}(H)$. Then for any $\sigma \ge 0$ with $e^{\sigma r}\psi, e^{\sigma r}H\psi \in \mathcal{H}$, one has $e^{\sigma r}\chi_\nu\psi \in \mathcal{D}(H)$ for all $\nu \ge 1$.*

Proof. Step I. We first claim $e^{\sigma r}\chi_{\nu,\nu'}\psi \in \mathcal{D}(H)$. Since $\psi \in \mathcal{H}^1$, we have

$$e^{\sigma r}\chi_{\nu,\nu'}\psi, e^{\sigma r}\chi_{\nu,\nu'}p\psi \in \mathcal{H},$$

and hence $pe^{\sigma r}\chi_{\nu,\nu'}\psi \in \mathcal{H}$ by (A.1). Choose a sequence $\psi_n \in C^\infty_c(\Omega)$ such that, as $n \to \infty$,

$$\|\psi - \psi_n\| + \|p(\psi - \psi_n)\| \to 0, \tag{A.7}$$

and then by (A.1) again, as $n \to \infty$,

$$e^{\sigma r}\chi_{\nu,\nu'}\psi_n \to e^{\sigma r}\chi_{\nu,\nu'}\psi, \quad pe^{\sigma r}\chi_{\nu,\nu'}\psi_n \to pe^{\sigma r}\chi_{\nu,\nu'}\psi \quad \text{in } \mathcal{H}.$$

This implies that $e^{\sigma r}\chi_{\nu,\nu'}\psi \in \mathcal{H}^1$. Note the distributional identity

$$He^{\sigma r}\chi_{\nu,\nu'}\psi = e^{\sigma r}\chi_{\nu,\nu'}H\psi - e^{\sigma r}(\sigma\chi_{\nu,\nu'} + \chi'_{\nu,\nu'})\partial^r\psi - \tfrac12(\Delta e^{\sigma r}\chi_{\nu,\nu'})\psi. \tag{A.8}$$

Then since $\psi, p\psi, H\psi \in \mathcal{H}$, and by (A.1)

$$\chi_\nu|\Delta r| = \tfrac{1}{2r}\chi_\nu|(\Delta r^2) - 2|\mathrm{d}r|^2| \le C, \tag{A.9}$$

we have $He^{\sigma r}\chi_{\nu,\nu'}\psi \in \mathcal{H}$. Hence $e^{\sigma r}\chi_{\nu,\nu'}\psi \in \mathcal{D}(H)$.

Step II. We next show $e^{\sigma r}\chi_\nu p\psi \in \mathcal{H}$. Noting that $e^{\sigma r}\chi_{\nu,\nu'}\psi \in \mathcal{H}^1$ as in Step I, we commute and estimate by Conditions A.1 and A.2

$$\begin{aligned}\|e^{\sigma r}\chi_{\nu,\nu'}p\psi\|^2 &= \|pe^{\sigma r}\chi_{\nu,\nu'}\psi\|^2 - \langle|\nabla e^{\sigma r}\chi_{\nu,\nu'}|^2 - \tfrac12(\Delta e^{2\sigma r}\chi^2_{\nu,\nu'})\rangle_\psi \\ &\le 4\langle H\rangle_{e^{\sigma r}\chi_{\nu,\nu'}\psi} + C_{1,\sigma}\|e^{\sigma r}\chi_{\nu/2,2\nu'}\psi\|^2.\end{aligned}$$

Whence, by reversing a commutation used above,

$$\begin{aligned}\|\mathrm{e}^{\sigma r}\chi_{\nu,\nu'}p\psi\|^2 &\le 4\mathrm{Re}\,\langle \mathrm{e}^{\sigma r}\chi_{\nu,\nu'}\psi, \mathrm{e}^{\sigma r}\chi_{\nu,\nu'}H\psi\rangle + C_{2,\sigma}\|\mathrm{e}^{\sigma r}\chi_{\nu/2,2\nu'}\psi\|^2\\ &\le \|\mathrm{e}^{\sigma r}\chi_{\nu,\nu'}H\psi\|^2 + C_\sigma\|\mathrm{e}^{\sigma r}\chi_{\nu/2,2\nu'}\psi\|^2\\ &\le \|\mathrm{e}^{\sigma r}\chi_{\nu}H\psi\|^2 + C_\sigma\|\mathrm{e}^{\sigma r}\chi_{\nu/2}\psi\|^2.\end{aligned}$$

Now we let $\nu'\to\infty$ invoking the Lebesgue dominated convergence theorem, and we conclude that $\mathrm{e}^{\sigma r}\chi_\nu p\psi\in\mathcal{H}$.

Step III. We note $p\mathrm{e}^{\sigma r}\chi_\nu\psi\in\mathcal{H}$ by Step II. We choose a sequence $\psi_n\in C^\infty_{\mathrm{c}}(\Omega)$ satisfying (A.7) as $n\to\infty$, and estimate

$$\|\mathrm{e}^{\sigma r}\chi_\nu\psi - \mathrm{e}^{\sigma r}\chi_{\nu,\nu'}\psi_n\| + \|p(\mathrm{e}^{\sigma r}\chi_\nu\psi - \mathrm{e}^{\sigma r}\chi_{\nu,\nu'}\psi_n)\|. \tag{A.10}$$

For $\nu'\ge 2\nu$ we have the first term of (A.10) bounded by

$$\|\mathrm{e}^{\sigma r}\chi_\nu\psi - \mathrm{e}^{\sigma r}\chi_{\nu,\nu'}\psi_n\| \le \|\mathrm{e}^{\sigma r}\chi_{\nu'}\psi\| + \|\mathrm{e}^{\sigma r}\chi_{\nu,\nu'}(\psi-\psi_n)\|,$$

and the second term bounded by

$$\begin{aligned}&\|p(\mathrm{e}^{\sigma r}\chi_\nu\psi - \mathrm{e}^{\sigma r}\chi_{\nu,\nu'}\psi_n)\|\\ &\le \|p\mathrm{e}^{\sigma r}\chi_{\nu'}\psi\| + \|p\mathrm{e}^{\sigma r}\chi_{\nu,\nu'}(\psi-\psi_n)\|\\ &\le \|\mathrm{e}^{\sigma r}\chi_{\nu'}p\psi\| + C_\sigma\|\mathrm{e}^{\sigma r}\chi_{\nu'/2,2\nu'}\psi\| + \|\mathrm{e}^{\sigma r}\chi_{\nu,\nu'}p(\psi-\psi_n)\| + C_\sigma\|\mathrm{e}^{\sigma r}\chi_{\nu/2,2\nu'}(\psi-\psi_n)\|.\end{aligned}$$

Thus we can make (A.10) arbitrarily small by letting ν' be large and then n large. Whence we obtain a sequence of states $\psi_{n(\cdot)}$ verifying

$$\|\mathrm{e}^{\sigma r}\chi_\nu\psi - \mathrm{e}^{\sigma r}\chi_{\nu,\nu'(m)}\psi_{n(m)}\| + \|p(\mathrm{e}^{\sigma r}\chi_\nu\psi - \mathrm{e}^{\sigma r}\chi_{\nu,\nu'(m)}\psi_{n(m)})\| \to 0$$

as $m\to\infty$, and hence $\mathrm{e}^{\sigma r}\chi_\nu\psi\in\mathcal{H}^1$.

Finally using the distributional identity

$$H\mathrm{e}^{\sigma r}\chi_\nu\psi = \mathrm{e}^{\sigma r}\chi_\nu H\psi - \mathrm{e}^{\sigma r}(\sigma\chi_\nu+\chi_\nu')\partial^r\psi - \tfrac12(\Delta\mathrm{e}^{\sigma r}\chi_\nu)\psi$$

we learn, cf. (A.8) and (A.9), that $H\mathrm{e}^{\sigma r}\chi_\nu\psi\in\mathcal{H}$ and hence that $\mathrm{e}^{\sigma r}\chi_\nu\psi\in\mathcal{D}(H)$. □

Corollary A.6. *Suppose $\psi\in\mathcal{D}(H)$ satisfies $\mathrm{e}^{\sigma r}\psi, \mathrm{e}^{\sigma r}H\psi\in\mathcal{H}$ for all $\sigma\ge 0$. Then for all $\sigma\ge0$ and $\nu\ge1$ one has $\mathrm{e}^{\sigma r}\chi_\nu\psi\in\mathcal{D}(H)\cap\mathcal{D}(A)$.*

A.3. **Undoing commutators.**

Lemma A.7. *For any $s\in[-1,1]$ the inclusion $\mathrm{e}^{\mathrm{i}tA}\mathcal{H}^s\subseteq\mathcal{H}^s$ holds, and*

$$\sup_{|t|<1}\|\mathrm{e}^{\mathrm{i}tA}\|_{\mathcal{B}(\mathcal{H}^s)}<\infty. \tag{A.11}$$

Moreover, $\mathrm{e}^{\mathrm{i}tA}\colon\mathcal{H}^s\to\mathcal{H}^s$ is strongly continuous in $t\in\mathbb{R}$.

Proof. Let us first set $s=1$. For any $\psi\in C^\infty_{\mathrm{c}}(\Omega)$ we can compute by (A.4)

$$\begin{aligned}&p_i(\mathrm{e}^{\mathrm{i}tA}\psi)(x)\\ &=\left(\int_0^t \tfrac12[p_i(\mathrm{e}^{2s}x)^j](\partial_j\Delta r^2)(\mathrm{e}^{2s}x)\,\mathrm{d}s\right)(\mathrm{e}^{\mathrm{i}tA}\psi)(x) + [\partial_i(\mathrm{e}^{2t}x)^j](\mathrm{e}^{\mathrm{i}tA}p_j\psi)(x).\end{aligned} \tag{A.12}$$

Here and below we slightly abuse notation writing $(\mathrm{e}^{\mathrm{i}tA}p_j\psi)(x)$ rather than $\mathrm{e}^{\int\cdots}(p_j\psi)(e^{2t}x)$. Then by (A.1) and Lemma A.4 for any $|t|\le T$

$$\begin{aligned}\|\mathrm{e}^{\mathrm{i}tA}\psi\|_{\mathcal{H}^1}^2 &= \|\psi\|_{\mathcal{H}}^2+\|p\mathrm{e}^{\mathrm{i}tA}\psi\|_{\mathcal{H}}^2\\ &\le \|\psi\|_{\mathcal{H}}^2+C_T\|\mathrm{e}^{\mathrm{i}tA}\psi\|_{\mathcal{H}}^2+C_T\|\mathrm{e}^{\mathrm{i}tA}p\psi\|_{\mathcal{H}}^2\\ &\le C_T\|\psi\|_{\mathcal{H}^1}^2.\end{aligned}$$

By a density argument this implies $\mathrm{e}^{\mathrm{i}tA}\mathcal{H}^1\subseteq\mathcal{H}^1$, and moreover for any $\psi\in\mathcal{H}^1$ and $|t|\le T$

$$\|\mathrm{e}^{\mathrm{i}tA}\psi\|_{\mathcal{H}^1}^2\le C_T\|\psi\|_{\mathcal{H}^1}^2.$$

Thus (A.11) follows for $s=1$. As for the strong continuity as $\mathcal{H}^1\to\mathcal{H}^1$, we can show it first on $C_{\mathrm{c}}^\infty(\Omega)$ using (A.12) and standard regularity properties for flows, and then extend it by the boundedness.

We can show the same results for $s=-1$ by taking the adjoint, and then the assertions are proved for $s\in(-1,1)$ by interpolation. □

Lemma A.8. *There exists $C>0$ such that for any $|t|<1$*

$$\|H\mathrm{e}^{\mathrm{i}tA}-\mathrm{e}^{\mathrm{i}tA}H\|_{\mathcal{B}(\mathcal{H}^1,\mathcal{H}^{-1})}\le C|t|$$

Proof. As a quadratic form on $C_{\mathrm{c}}^\infty(\Omega)$, or as an operator $C_{\mathrm{c}}^\infty(\Omega)\to\mathcal{H}^{-1}$,

$$\begin{aligned}H\mathrm{e}^{\mathrm{i}tA}-\mathrm{e}^{\mathrm{i}tA}H &= \int_0^t \tfrac{\mathrm{d}}{\mathrm{d}s}\mathrm{e}^{\mathrm{i}(t-s)A}H\mathrm{e}^{\mathrm{i}sA}\,\mathrm{d}s\\ &= \int_0^t \mathrm{e}^{\mathrm{i}sA}\mathrm{i}[H,A]\mathrm{e}^{\mathrm{i}(t-s)A}\,\mathrm{d}s.\end{aligned}$$

Then by Lemma A.7 and the density of $C_{\mathrm{c}}^\infty(\Omega)\subseteq\mathcal{H}^1$ the assertion follows. □

Lemma A.9. *The following strong limit to the right exists in $\mathcal{B}(\mathcal{H}^1,\mathcal{H}^{-1})$, and the following equality holds*

$$\mathrm{i}[H,A]=\operatorname*{s-lim}_{t\to0}t^{-1}[H\mathrm{e}^{\mathrm{i}tA}-\mathrm{e}^{\mathrm{i}tA}H]. \tag{A.13}$$

Proof. For any $\psi\in C_{\mathrm{c}}^\infty(\Omega)$

$$t^{-1}(H\mathrm{e}^{\mathrm{i}tA}-\mathrm{e}^{-\mathrm{i}tA}H)\psi-\mathrm{i}[H,A]\psi=t^{-1}\int_0^t\bigl\{\mathrm{e}^{\mathrm{i}sA}\mathrm{i}[H,A]\mathrm{e}^{\mathrm{i}(t-s)A}-\mathrm{i}[H,A]\bigr\}\psi\,\mathrm{d}s.$$

We use the strong continuity of $\mathrm{e}^{\mathrm{i}tA}$ of Lemma A.7 to obtain (A.13) on $C_{\mathrm{c}}^\infty(\Omega)$. Then by Lemma A.8 and the density argument, the strong limit of (A.13) exists in $\mathcal{B}(\mathcal{H}^1,\mathcal{H}^{-1})$. □

The following lemma is a main result of this appendix:

Lemma A.10. *Suppose $\psi\in\mathcal{D}(H)$ satisfies $\mathrm{e}^{\sigma r}\psi,\mathrm{e}^{\sigma r}H\psi\in\mathcal{H}$ for all $\sigma\ge0$. Then for all $\sigma\ge0$ and $\nu\ge1$*

$$\langle\mathrm{i}[H,A]\rangle_{\mathrm{e}^{\sigma r}\chi_\nu\psi}=\mathrm{i}\langle H\mathrm{e}^{\sigma r}\chi_\nu\psi,A\mathrm{e}^{\sigma r}\chi_\nu\psi\rangle-\mathrm{i}\langle A\mathrm{e}^{\sigma r}\chi_\nu\psi,H\mathrm{e}^{\sigma r}\chi_\nu\psi\rangle.$$

Proof. We note $\mathrm{e}^{\sigma r}\chi_\nu\psi\in\mathcal{D}(H)\cap\mathcal{D}(A)$ by Corollary A.6. Then, by Lemma A.9

$$\begin{aligned}\langle\mathrm{i}[H,A]\rangle_{\mathrm{e}^{\sigma r}\chi_\nu\psi}&=\lim_{t\to0}\langle t^{-1}[H\mathrm{e}^{\mathrm{i}tA}-\mathrm{e}^{\mathrm{i}tA}H]\rangle_{\mathrm{e}^{\sigma r}\chi_\nu\psi}\\ &=\mathrm{i}\langle H\mathrm{e}^{\sigma r}\chi_\nu\psi,A\mathrm{e}^{\sigma r}\chi_\nu\psi\rangle-\mathrm{i}\langle A\mathrm{e}^{\sigma r}\chi_\nu\psi,H\mathrm{e}^{\sigma r}\chi_\nu\psi\rangle.\end{aligned}$$

□

A.4. **Examination of** (3.13a)**,** (3.13b) **and** (3.26)**.** It is easy to prove (3.13a) by Lemma A.7 for $s = 1$ combined with the smallness of V, cf. Condition A.1. Similarly (3.26) is a consequence of Lemma A.9. The bound (3.13b) is already obtained by the explicit formula $\|p_r \mathrm{e}^{\mathrm{i}tA}\psi\| = \mathrm{e}^{2t}\|p_r\psi\|$, but below we show a more general result involving in fact only parts of Condition A.2. This is for the quadratic form $P_r^* P_r$ where $P_r = \frac{1}{2}\big(p^r + (p^r)^*\big)$ is the operator closure of this action on $C_\mathrm{c}^\infty(\Omega)$. Whence in particular $P_r^* P_r$ is closed on $Q(P_r^* P_r) = \mathcal{D}(P_r)$.

Lemma A.11. *Suppose* (Ω, g) *is a Riemannian manifold of dimension* $d \geq 1$ *for which there exists a real-valued function* $r \in C^\infty(\Omega)$ *obeying Condition A.2 (1) and the bounds*

$$\sup |\mathrm{d}r| < \infty, \quad \sup |\partial^r |\mathrm{d}r|^2| < \infty.$$

Then the inclusion $\mathrm{e}^{\mathrm{i}tA}\mathcal{D}(P_r) \subseteq \mathcal{D}(P_r)$ *holds, and*

$$\sup_{|t|<1} \|\mathrm{e}^{\mathrm{i}tA}\|_{\mathcal{B}(\mathcal{D}(P_r))} < \infty. \tag{A.14}$$

Proof. We first note that

$$\partial_t r(\mathrm{e}^{2t}x) = 2r(\mathrm{e}^{2t}x)(\partial^r r)(\mathrm{e}^{2t}x) = 2r(\mathrm{e}^{2t}x)|\mathrm{d}r(\mathrm{e}^{2t}x)|^2,$$

and this implies

$$r(\mathrm{e}^{2t}x) = r(x) \exp\left(2\int_0^t |\mathrm{d}r(\mathrm{e}^{2s}x)|^2 \,\mathrm{d}s\right). \tag{A.15}$$

Let $\psi \in C_\mathrm{c}^\infty(M)$. Then, by $A\mathrm{e}^{\mathrm{i}tA}\psi = \mathrm{e}^{\mathrm{i}tA}A\psi$ and $A = 2rP_r + \frac{1}{\mathrm{i}}|\mathrm{d}r|^2$, we can compute

$$\begin{aligned}
&r(x)(P_r\mathrm{e}^{\mathrm{i}tA}\psi)(x)\\
&= (\mathrm{e}^{\mathrm{i}tA}rP_r\psi)(x) - \tfrac{\mathrm{i}}{2}\big(|\mathrm{d}r(\mathrm{e}^{2t}x)|^2 - |\mathrm{d}r(x)|^2\big)(\mathrm{e}^{\mathrm{i}tA}\psi)(x)\\
&= r(\mathrm{e}^{2t}x)(\mathrm{e}^{\mathrm{i}tA}P_r\psi)(x) - \tfrac{\mathrm{i}}{2}\left(\int_0^t \partial_s|\mathrm{d}r(\mathrm{e}^{2s}x)|^2\,\mathrm{d}s\right)(\mathrm{e}^{\mathrm{i}tA}\psi)(x)\\
&= r(\mathrm{e}^{2t}x)(\mathrm{e}^{\mathrm{i}tA}P_r\psi)(x) - \mathrm{i}\left(\int_0^t r(\mathrm{e}^{2s}x)(\partial^r|\mathrm{d}r|^2)(\mathrm{e}^{2s}x)\,\mathrm{d}s\right)(\mathrm{e}^{\mathrm{i}tA}\psi)(x),
\end{aligned}$$

so that we obtain using (A.15)

$$|(P_r\mathrm{e}^{\mathrm{i}tA}\psi)(x)| \leq C_T\big(|(\mathrm{e}^{\mathrm{i}tA}P_r\psi)(x)| + |(\mathrm{e}^{\mathrm{i}tA}\psi)(x)|\big) \tag{A.16}$$

for $|t| < T$ and $x \notin r^{-1}(0)$. By continuity (A.16) remains valid for $|t| < T$ and x in the boundary of $r^{-1}(0)$. On the other hand for any interior point x of $r^{-1}(0)$ we compute using (A.4) and that $\mathrm{e}^{2s}x = x$,

$$\begin{aligned}
(\mathrm{e}^{\mathrm{i}tA}\psi)(x) &= \psi(x),\\
(P_r\mathrm{e}^{\mathrm{i}tA}\psi)(x) &= P_r\psi(x) = (\mathrm{e}^{\mathrm{i}tA}P_r\psi)(x).
\end{aligned}$$

The latter formula agrees with (A.16) for $|t| < T$, and it follows that (A.16) is valid uniformly in $x \in \Omega$ and $|t| < T$. Consequently

$$\|\mathrm{e}^{\mathrm{i}tA}\psi\|^2_{\mathcal{D}(P_r)} \leq C_T\|\psi\|^2_{\mathcal{D}(P_r)}.$$

We complete the proof by a density argument. $\square$

Appendix B

In this appendix we introduce the notion of strictly convexity of an obstacle and derive the geometric properties needed for the one-body type model considered in Subsection 3.2.

Let $\Theta \subset \mathbb{R}^d$, $d \geq 2$, be a bounded open set, denote its closure by $\overline{\Theta}$, and set $\Omega = \mathbb{R}^d \setminus \overline{\Theta}$. The goal of these short notes is to give a criterion for the existence of a function $r \in C^\infty(\Omega)$ such that for some $c > 0$

$$|\nabla r| = 1 \text{ in } \Omega, \tag{B.1a}$$

$$(\nabla^2 r)_{|S_r} \geq c\langle r\rangle^{-1} g_{|S_r}, \tag{B.1b}$$

$$|\partial^\gamma r| \leq C_\alpha \langle r\rangle^{1-|\gamma|}, \tag{B.1c}$$

where g is the Euclidean metric, $S_r = r^{-1}(r)$ is the level surface and $g_{|S_r}$ is the pull-back of g to S_r. Note that S_r is smooth by (B.1a). We impose the following convexity type condition for Θ. Note that the inequality (B.1b) represents the convexity of r.

Condition B.1. Let $\Theta \subset \mathbb{R}^d$, $d \geq 2$, be an open connected subset with smooth boundary $S = \partial\Theta$, and $\nu \in \Gamma(N^+S)$ be the outward unit normal vector field on S. There exists a constant $\kappa > 0$ such that

$$(\nabla \nu)_{|S} \geq \kappa g_{|S}. \tag{B.2}$$

A subset $\Theta \subset \mathbb{R}^d$ fulfilling Condition B.1 is called *strictly convex*. We show in Lemma B.4 that such set is convex. The symmetric tensor $(\nabla\nu)_{|S}$ is called the *second fundamental form* of S, and its eigenvalues relative to $g_{|S}$ are called the *principal curvatures*. Hence (B.2) implies that the principal curvatures are bounded below by $\kappa > 0$. For these notions we refer to [Cha, Section II.2], although we adopt different signs for them.

Proposition B.2. *Suppose $\Theta \subset \mathbb{R}^d$ is strictly convex. Then the distance function $r(x) = \operatorname{dist}(x, \Theta)$, $x \in \Omega$, satisfies (B.1a)–(B.1c).*

In the sequel we prove Proposition B.2. We first show the convexity of Θ.

Lemma B.3. *Let $x \in S$ and set $\tilde{S}_x = \exp[(TS)_x]$. Then there exists a neighborhood U of x in $\mathbb{R}^d$ such that $\overline{\Theta} \cap \tilde{S}_x \cap U = \{x\}$.*

This is a sort of *local convexity*. We omit the proof, just referring to [Cha, Exercise II.4].

Lemma B.4. *For any $x, y \in \Theta$ the geodesic γ_{xy} connecting x and y lies in Θ.*

Proof. Let us argue by contradiction assuming the set

$$\Phi = \{(x, y) \in \Theta \times \Theta \,|\, \gamma_{xy}([0, 1]) \subset \Theta\}$$

does not coincide with $\Theta \times \Theta$. Since $\gamma_{xy}(t)$ is continuously dependent on (t, x, y), it is clear that Φ is open in $\Theta \times \Theta$. Since $\Theta \times \Theta$ is connected the boundary $\partial\Phi \subset \Theta \times \Theta$ is non-empty, so we can choose $(x, y) \in \partial\Phi$. Then by definition

$$\{0, 1\} \subset \mathcal{U} := \gamma_{xy}^{-1}(\Theta) \subsetneq [0, 1].$$

Clearly $\mathcal{U}$ is open in $[0, 1]$. We claim that $\mathcal{U}$ is also closed in $[0, 1]$ yielding the contradiction. For any $\tau \in [0, 1] \setminus \mathcal{U}$ the point $\gamma_{xy}(\tau) \in S$ and the geodesic γ_{xy} is tangent to S at $\gamma_{xy}(\tau)$ (here we use that $(x, y) \in \partial\Phi$). By Lemma B.3 we then conclude that $\tau' \notin \mathcal{U}$ for all τ' close to τ. $\square$

Now we are ready to give the distorted spherical coordinates for Ω.

Lemma B.5. *The exponential map on the outward normal vectors on S:*

$$\exp_{|N^+S}\colon N^+S \to \Omega$$

is bijective.

Proof. We shall intensively use the convexity of $\overline{\Theta}$. Let us denote an element of N^+S by $r\nu(\sigma)$, $(r,\sigma) \in (0,\infty) \times S$. If $\exp(r\nu(\sigma)) \in \overline{\Theta}$ for some (r,σ), then by the convexity this contradicts the fact that ν is outward. Thus the image $\exp(N^+S)$ is included in Ω.

Next, assume $\exp(r\nu(\sigma)) = \exp(r'\nu(\sigma'))$ for some (r,σ), (r',σ'). By the convexity we note that the obstacle Θ is in one side of the half space devided by the tangent plane at σ, and by the normality of $\nu(\sigma)$ we obtain $\mathrm{dist}(\exp(r\nu(\sigma)),\Theta) = r$. Thus $r = r'$. Moreover, by the convexity of $\overline{\Theta}$ and the minimality of $r = r' = \mathrm{dist}(\exp(r\nu(\sigma)),\Theta)$, $\sigma = \sigma'$.

Finally take any $x \in \Omega$, and then we can find $y \in \partial\Theta$ such that $\mathrm{dist}(x,\Theta) = \|x-y\|$. Then the geodesic connecting x and y is orthogonal to $\partial\Theta$, because, otherwise, $\|x-y\|$ does not give a minimal distance. This implies x is in the image $\exp(N^+S)$. □

As in the proof above we identify $N^+S \cong (0,\infty)\times S$ through

$$N^+S \ni r\nu(\sigma) \leftrightarrow (r,\sigma) \in (0,\infty)\times S,$$

and consider $(r,\sigma) \in (0,\infty)\times S$ as local coordinates of N^+S. By Lemma B.5 $\exp_{|N^+S}\colon N^+S \to \Omega$ is a C^∞ bijection, and r is well-defined as the distance function on Ω: $r(x) = \mathrm{dist}(x,\Theta)$, $x \in \Omega$. The following lemma implies that the pair (r,σ) in fact defines local coordinates for Ω.

Lemma B.6. *The exponential map $\exp_{|N^+S}\colon N^+S \to \Omega$ is a diffeomorphism.*

Proof. Parts of the arguments below depend on [Cha, Section III.6]. By Lemma B.5 it suffices to show that $\exp_{|N^+S}$ is a local diffeomorphism. For $r \geq 0$ and $\sigma \in S$ let $\gamma(\cdot;r,\sigma)$ be the geodesic defined by

$$\gamma(t;r,\sigma) = \exp(tr\nu(\sigma)), \quad t \in [0,1],$$

and we consider the vector field Y_α along it:

$$Y_\alpha(t) = \partial_\alpha\gamma(t;r,\sigma); \quad \partial_\alpha = \partial_{\sigma^\alpha},\ \alpha = 2,\dots,d.$$

The vector field Y_α is the so-called *Jacobi field* and satisfies the equation

$$\nabla^2_{\gamma'}Y_\alpha + R(\gamma',Y_\alpha)\gamma' = 0 \tag{B.3}$$

with the initial conditions

$$Y_\alpha(0) = \partial_\alpha, \quad (\nabla_{\gamma'}Y_\alpha)(0) = \pi_{(TS)_\sigma}(r\nabla_\alpha\nu). \tag{B.4}$$

Let $X_\alpha(t)$ be the parallel transport of $\partial_\alpha \in (TS)_\sigma$ along γ, i.e.

$$(\nabla_{\gamma'}X_\alpha)(t) = 0, \quad X_\alpha(0) = \partial_\alpha,$$

and seek for a solution to (B.3) and (B.4) of the form $Y_\alpha(t) = c_\alpha^\beta(t)X_\beta(t)$. Since $R = 0$ and $(\nabla_\alpha\nu)_\beta = ((\nabla^2 r)_{|S})_{\alpha\beta}$, we have (B.3) and (B.4) reduced to

$$(c_\alpha^\beta)''(t) = 0, \quad c_\alpha^\beta(0) = \delta_{\alpha\beta}, \quad (c_\alpha^\beta)'(0) = r((\nabla^2 r)_{|S})_{\alpha\gamma}(g_{|S})^{\gamma\beta}.$$

We can solve this as a matrix equation, and hence obtain

$$Y_\alpha(t) = X_\alpha(t) + tr((\nabla^2 r)_{|S})_{\alpha\gamma}(g_{|S})^{\gamma\beta}X_\beta(t). \tag{B.5}$$

Note that we can choose local coordinates σ such that ∂_α, $\alpha = 2, \dots, d$, are principal directions of S, so that $(\nabla^2 r)_{|S}$ and $g_{|S}$ are written as diagonal matrices. Then by the positivity (B.2) it is straightforward to see that the set of tangents $\{Y_\alpha(t) \,|\, \alpha = 2, \dots, d\}$ is linearly independent for all $t \geq 0$. Thus $\exp_{|N^+S}$ is a local diffeomorphism. □

Proof of Proposition B.2. By (B.5) we can write the metric of Ω in terms of coordinates (r, σ), and

$$g = \mathrm{d}r \otimes \mathrm{d}r + (g_{|S} + r(\nabla^2 r)_{|S})_{\alpha\gamma}(g_{|S})^{\gamma\delta}(g_{|S} + r(\nabla^2 r)_{|S})_{\delta\beta}\, \mathrm{d}\sigma^\alpha \otimes \mathrm{d}\sigma^\beta. \tag{B.6}$$

This can be verified by choosing local coordinates σ^α diagonalizing $(\nabla^2 r)_{|S}$ and $g_{|S}$ and using the fact that the parallel transport does not change the length of vectors. Now we recall that in general for a metric of the form

$$g = \mathrm{d}r \otimes \mathrm{d}r + h_{\alpha\beta}(r, \sigma)\mathrm{d}\sigma^\alpha \otimes \mathrm{d}\sigma^\beta$$

we can compute the Christoffel symbols $\Gamma^m_{ij} = \frac{1}{2} g^{km}\left(\frac{\partial}{\partial x^i} g_{kj} + \frac{\partial}{\partial x^j} g_{ik} - \frac{\partial}{\partial x^k} g_{ij}\right)$:

$$\Gamma^r_{rr} = 0, \quad \Gamma^r_{r\alpha} = 0, \quad \Gamma^\alpha_{rr} = 0, \quad \Gamma^r_{\alpha\beta} = -\tfrac{1}{2}\tfrac{\partial}{\partial r} h_{\alpha\beta}, \quad \Gamma^\alpha_{r\beta} = \tfrac{1}{2} h^{\alpha\gamma}\tfrac{\partial}{\partial r} h_{\gamma\beta}, \tag{B.7}$$

and hence

$$(\nabla^2 r)_{\alpha\beta} = -\Gamma^r_{\alpha\beta} = \tfrac{1}{2}\tfrac{\partial}{\partial r} h_{\alpha\beta}. \tag{B.8}$$

Applying (B.8) to the representation (B.6) we obtain

$$(\nabla^2 r)_{\alpha\beta} = ((\nabla^2 r)_{|S})_{\alpha\beta} + r((\nabla^2 r)_{|S})_{\alpha\gamma}(g_{|S})^{\gamma\delta}((\nabla^2 r)_{|S})_{\delta\beta}.$$

Then for any $c < 1$ there exists $r_0 > 0$ such that for all $r \geq r_0$

$$(\nabla^2 r)_{|S_r} \geq c r^{-1} g_{|S_r}.$$

Hence we have (B.1b).

We next prove (B.1c). Note the coordinate-free expression:

$$\sum_{|\gamma|=k} |\partial^\gamma r|^2 = |\nabla^k r|^2 = g^{i_1 j_1} \cdots g^{i_k j_k} (\nabla^k r)_{i_1 \cdots i_k} (\nabla^k r)_{j_1 \cdots j_k},$$

where ∂^γ to the left denotes the derivative in the Euclidean coordinates. Thus we can compute it in the (r, σ)-coordinates. By (B.6) we have

$$g^{rr} = O(1), \quad g^{\alpha\beta} = O(\langle r \rangle^{-2}), \quad g^{r\alpha} = g^{\alpha r} = 0,$$

and it suffices to show that in these coordinates $(\nabla^k r)_{i_1 \cdots i_k} = O(\langle r \rangle^{1-l})$, where l is the total number of occurrences of the subscript r in $\{i_1, \dots, i_k\}$. But this follows from the following stronger property:

$$\partial_{j_1} \cdots \partial_{j_s} (\nabla^k r)_{i_1 \cdots i_k} = O(\langle r \rangle^{1-l}),$$

where l is the total number of occurrences of the subscript r in $\{j_1, \dots, j_s\} \cup \{i_1, \dots, i_k\}$. The latter statement follows in turn by induction employing a standard recurrence formula for covariant derivatives (see for example [IS1]) and the expressions (B.6) and (B.7). Note that the statement is trivial for $k = 1$ and that it follows from (B.6) and (B.7) that

$$\partial_{j_1} \cdots \partial_{j_s} \Gamma^r_{\alpha\beta} = O(\langle r\rangle^{1-l}),$$
$$\partial_{j_1} \cdots \partial_{j_s} \Gamma^\eta_{\alpha\beta} = O(\langle r\rangle^{-l}),$$
$$\partial_{j_1} \cdots \partial_{j_s} \Gamma^\alpha_{r\beta} = O(\langle r\rangle^{-1-l}).$$

Here l denotes the number of occurrences of the subscript r in $\{j_1, \dots, j_s\}$ and $r \notin \{\alpha, \beta, \eta\}$. These bounds and the recurrence formula suffice for the induction step by the Leibniz rule for differentiation. □

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