Available online at www.sciencedirect.com

SciVerse ScienceDirect

Journal of Functional Analysis 264 (2013) 1929–1974

JOURNAL OF Functional Analysis

www.elsevier.com/locate/jfa

Scattering theory for Riemannian Laplacians ☆

K. Ito [a,*], E. Skibsted [b]

[a] *Graduate School of Pure and Applied Sciences, University of Tsukuba, 1-1-1 Tennodai, Tsukuba, Ibaraki 305-8571, Japan*

[b] *Institut for Matematiske Fag, Aarhus Universitet, Ny Munkegade 8000 Aarhus C, Denmark*

Received 16 August 2012; accepted 1 February 2013

Available online 11 February 2013

Communicated by I. Rodnianski

Abstract

We introduce a notion of scattering theory for the Laplace–Beltrami operator on non-compact, connected and complete Riemannian manifolds. A principal condition is given by a certain positive lower bound of the second fundamental form of angular submanifolds at infinity. Another condition is certain bounds of derivatives up to order one of the trace of this quantity. These conditions are shown to be optimal for existence and completeness of a wave operator. Our theory does not involve prescribed asymptotic behavior of the metric at infinity (like asymptotic Euclidean or hyperbolic metrics studied previously in the literature). A consequence of the theory is spectral theory for the Laplace–Beltrami operator including identification of the continuous spectrum and absence of singular continuous spectrum.

Keywords: Scattering theory; Schrödinger operators; Riemannian manifold; Spectral theory

Contents

1. Introduction and results 1930
   1.1. Uniqueness of the wave operator 1936
   1.2. Manifold with a pole 1937

☆ This work was essentially done during K.I.'s stay in Aarhus University (academic year 2009–2010). He would like to express his gratitude for financial support from FNU 160377 (2009–2011) as well as from JSPS Wakate (B) 21740090 (2009–2012). E.S. thanks H.D. Cornean and I. Herbst for many preliminary discussions of scattering theory on manifolds [4]. We thank H. Kumura for bringing our attention on his work [19].

* Corresponding author.
E-mail addresses: ito-ken@math.tsukuba.ac.jp (K. Ito), skibsted@imf.au.dk (E. Skibsted).

0022-1236/$ – see front matter
http://dx.doi.org/10.1016/j.jfa.2013.02.002

2. Geometric setting considerations . . . 1939
2.1. Examples . . . 1939
2.2. Counter examples, borderlines of conditions . . . 1942
2.3. Classical Mechanics under Conditions 1.9 and 1.2 . . . 1945
3. Reduction of the proof of Theorem 1.5 . . . 1948
3.1. Reduction to existence of localization operators . . . 1948
3.2. Localization operators in explicit form . . . 1952
4. Verification of properties of localization operators . . . 1954
4.1. Commutator computations . . . 1954
4.2. Further commutator computations . . . 1958
4.3. Proof of Lemma 3.1 . . . 1961
4.4. Preliminary localization for perturbed dynamics . . . 1963
4.5. Proof of Lemma 3.2 . . . 1973
References . . . 1973

1. Introduction and results

In this paper we introduce a notion of scattering theory for the Laplace–Beltrami operator on a rather general type of non-compact manifold. In particular we do not impose asymptotics of the metric at infinity. Immediate consequences include identification of the continuous spectrum and absence of singular continuous spectrum. We also show that our wave operator implements a certain family of commuting asymptotic observables. To our knowledge most previous works on spectral and scattering theory for the Laplace–Beltrami operator on manifolds require asymptotics of the metric at infinity (or at least asymptotics of the large ball volume), see for example [1,8,10,15,18–21]. Among these works probably [8] is the closest to our setup. In fact Donnelly's assumptions include the existence of a certain *exhaustion function* b resembling the function r appearing in our assumptions, see Conditions 1.2 and 1.3 below. However he needs asymptotics of the Hessian of b^2 while our Condition 1.2 is a lower bound only of the Hessian of the analogous function r^2. Moreover the main issue of our paper is scattering theory while [8] only deals with spectral theory. In a companion paper [16] we prove absence of embedded eigenvalues under weaker conditions than considered in the present paper. All of our results generalize to Schrödinger operators on manifolds (with short-range potentials). We state and prove our results in this more general context.

The comparison dynamics used to define our wave operator is constructed from a certain family of geodesics for the (full) metric in the spirit of primarily [14,3]. In this sense it is non-perturbatively constructed. Nevertheless it provides a simple explicit description of the large time behavior of continuous spectrum wave packets which is a fundamental goal of scattering theory [6].

Let (M, g) be a connected complete d-dimensional Riemannian manifold, $d \geqslant 2$. In the present paper we discuss the scattering theory for the Schrödinger operator

$$H = -\frac{1}{2}\Delta + V = H_0 + V \tag{1.1}$$

on the Hilbert space $\mathcal{H} = L^2(M) = L^2(M, (\det g)^{1/2}\,\mathrm{d}x)$. Here Δ is the Laplace–Beltrami operator: In any local coordinates x, if $g = g_{ij}\,\mathrm{d}x^i \otimes \mathrm{d}x^j$, then

$$-\Delta = p_i^* g^{ij} p_j = \frac{1}{(\det g)^{1/2}} p_i (\det g)^{1/2} g^{ij} p_j, \qquad p_i = -\mathrm{i}\partial_i.$$

Note that indeed $p_i^* = (\det g)^{-1/2} p_i (\det g)^{1/2}$ is the adjoint of p_i. Since our conditions will include that the potential $V = V(x)$ is bounded (Condition 1.4 given below states that it is bounded and short-range) $H = H_0 + V$ is essentially self-adjoint on $C_c^\infty(M)$. Concerning geometric notions appearing below we refer to [2] (see also [17] or [22]).

We first impose, cf. [18],

Condition 1.1. There exists a relatively compact open set $O \Subset M$ such that the boundary ∂O is smooth and the exponential map restricted to outward normal vectors: $\exp : N^+\partial O \to E := M \setminus \overline{O}$ is diffeomorphic.

Then we call a component of E an *end* and such M a *manifold with ends*.

The distance function $r(x) = \mathrm{dist}(x, \partial O)$, $x \in E$, belongs to $C^\infty(E)$. In a neighborhood of ∂O, say $\mathcal{O}$, we have an extension of r, say $\tilde{r}$, with the property $\tilde{r} \in C^\infty(\mathcal{O})$. In fact we can choose this extension as the "signed distance function". We can then construct an extension $\tilde{r} \in C^\infty(M)$ for which we may assume (although these requirements are not essential) $-1 \leqslant \tilde{r} < 0$ and $|\nabla\tilde{r}| \leqslant 1$ on O (this is by considering a certain composition of functions). In the following we use the notation r for this extended function. We point out that our main results will be independent of the extension procedure, however we prefer in proofs to work entirely with objects defined on the whole of M (rather than with some defined on E only).

We denote the Levi-Civita connection on TM by $\nabla : \Gamma(TM) \to \Gamma(TM \otimes T^*M)$. In general, the connection ∇ extends naturally to

$$\nabla : \Gamma\big((TM)^{\otimes p} \otimes \big(T^*M\big)^{\otimes q}\big) \to \Gamma\big((TM)^{\otimes p} \otimes \big(T^*M\big)^{\otimes (q+1)}\big)$$

in the following way (cf. [2, p. 31]): For any

$$t = \big(t^{i_1\cdots i_p}_{j_1\cdots j_q}\big) \in \Gamma\big((TM)^{\otimes p} \otimes \big(T^*M\big)^{\otimes q}\big)$$

$\nabla t \in \Gamma((TM)^{\otimes p} \otimes (T^*M)^{\otimes (q+1)})$ is given by

$$(\nabla t)^{i_1\cdots i_p}_{j_0 j_1\cdots j_q} = \partial_{j_0} t^{i_1\cdots i_p}_{j_1\cdots j_q} + \sum_{s=1}^{p} \Gamma^{i_s}_{j_0 k} t^{i_1\cdots i_{s-1} k i_{s+1}\cdots i_p}_{j_1\cdots j_q} - \sum_{s=1}^{q} \Gamma^k_{j_0 j_s} t^{i_1\cdots i_p}_{j_1\cdots j_{s-1} k j_{s+1}\cdots j_q},$$

where $\Gamma^k_{ij} = 2^{-1} g^{kl}(\partial_i g_{lj} + \partial_j g_{li} - \partial_l g_{ij})$ are the Christoffel symbols. For example, it follows that $\nabla r^2 = \mathrm{d}r^2 \in \Gamma(T^*M)$ and $\nabla^2 r^2 = \nabla\nabla r^2 \in \Gamma(T^*M \otimes T^*M)$. The operator ∇^2 gives the geometric Hessian, and in local coordinates

$$\big(\nabla^2 r^2\big)_{ij} = \partial_i\partial_j r^2 - \Gamma^k_{ij}\partial_k r^2. \tag{1.2}$$

We note that $(\nabla^2 r^2)_{ij}$ are the coefficients of the principal part of a Mourre type commutator, cf. Corollary 4.2 and Lemma 4.12 (for the analogous statement in Classical Mechanics see the end of Subsection 2.3).

Condition 1.2 *(Mourre type condition).* There exist $\delta \in (0, 1]$ and $r_0 \geqslant 0$ such that

$$\nabla^2 r^2 \geqslant (1+\delta) g \quad \text{for } r \geqslant r_0. \tag{1.3}$$

Note that (1.3) is an inequality of quadratic forms on fibers of TM. The condition (1.3) can also be formulated in terms of the second fundamental form of the *angular manifolds* $S_r = \{x \in E;\ r(x) = r\} \cong \partial O$. We let $\iota_r : S_r \hookrightarrow M$ be the inclusion and $\mathrm{D} = \iota_r^* \circ \nabla$ (cf. [2, Proposition 2.3]). Then (1.3) is equivalent to the following inequality in the sense of quadratic forms on TS_r:

$$\mathrm{D}\nabla r \geqslant \frac{(1+\delta)}{2r} \iota_r^* g \quad \text{for } r > r_0. \tag{1.4}$$

In fact, a computation in the geodesic spherical coordinates shows that

$$\nabla^2 r^2 = 2\mathrm{d}r \otimes \mathrm{d}r \oplus 2r\mathrm{D}\nabla r, \qquad g = \mathrm{d}r \otimes \mathrm{d}r \oplus \iota_r^* g. \tag{1.5}$$

Here the direct sum decompositions correspond to the orthogonal splitting $TM_x \cong (NS_r)_x \oplus (TS_r)_x$ at any point $x \in S_r$.

As we can see from (1.2) the inequality (1.3) is a condition on derivatives of the metric tensor g up to first order (as well as on derivatives of the function r^2 of course). The condition (1.6a) below is on derivatives up to second order.

Condition 1.3 *(Quantum mechanics bound).* There exists $\kappa \in (0, 1/2)$ such that

$$\left|\mathrm{d}\Delta r^2\right| \leqslant C\langle r\rangle^{-1/2-\kappa}. \tag{1.6a}$$

We used the standard notation $\langle r\rangle = (1+r^2)^{1/2}$. Due to (1.11) given below we have $\partial_i \Delta r^2 = g^{jk}(\nabla^3 r^2)_{ijk}$. We notice that it is a consequence of Condition 1.3 that

$$\Delta r = O\bigl(r^{-1/2-\kappa}\bigr) \quad \text{and} \quad |\mathrm{d}\Delta r| = O\bigl(r^{-3/2-\kappa}\bigr), \tag{1.6b}$$

in fact (1.6a) and (1.6b) are equivalent for any $\kappa \in (0, 1/2)$. Whence yet another equivalent condition (given in terms of the mean curvature) is

$$\mathrm{tr}(\mathrm{D}\nabla r) = O\bigl(r^{-1/2-\kappa}\bigr) \quad \text{and} \quad \left|\mathrm{d}\,\mathrm{tr}(\mathrm{D}\nabla r)\right| = O\bigl(r^{-3/2-\kappa}\bigr). \tag{1.6c}$$

The first bound of (1.6c) implies an upper bound of the ball volume growth of the form $\exp(Cr^{1/2-\kappa})$, $C > 0$, and in general no better. Similarly Condition 1.2 implies the power type lower bound of the ball volume growth cr^{σ} with $\sigma = (\delta+1)(d-1)/2 + 1$ and $c > 0$.

In the analysis of the Classical Mechanics in Subsection 2.3 we do not need Condition 1.3.

Finally we impose a short-range condition on V:

Condition 1.4. The potential $V \in L^\infty(M;\mathbb{R})$ satisfies for some $\eta \in (0,1]$

$$\left|V(x)\right| \leqslant C\langle r\rangle^{-1-\eta}. \tag{1.7}$$

Under the above setting we prove the existence and the completeness of the wave operator. Define the free propagator $U(t)$, $t>0$, by

$$U(t) = \mathrm{e}^{\mathrm{i}K(t,\cdot)}\mathrm{e}^{-\mathrm{i}\frac{\ln t}{2}A}; \tag{1.8a}$$

$$K(t,x) = \frac{r(x)^2}{2t}, \tag{1.8b}$$

$$A = \mathrm{i}\left[H_0, r^2\right] = \frac{1}{2}\left\{\left(\partial_i r^2\right)g^{ij}p_j + p_i^* g^{ij}\left(\partial_j r^2\right)\right\}. \tag{1.8c}$$

Here $\mathrm{e}^{-\mathrm{i}\frac{\ln t}{2}A}$ is called a dilation with respect to r. If we define a flow $\omega = \omega(t,x)$, $(t,x) \in (0,\infty)\times M$, by

$$\partial_t \omega^i = -\frac{1}{2t}g^{ij}(\omega)\left(\partial_j r^2\right)(\omega), \qquad \omega(1,x) = x, \tag{1.9}$$

then for $u \in \mathcal{H}$

$$\mathrm{e}^{-\mathrm{i}\frac{\ln t}{2}A}u(x) = J\left(\omega(t,x)\right)^{1/2}\left(\frac{\det g(\omega(t,x))}{\det g(x)}\right)^{1/4}u\left(\omega(t,x)\right), \tag{1.10}$$

where J is the relevant Jacobian. In fact, using (1.9) and the relation

$$\Delta u = \operatorname{tr}\left(\nabla^2 u\right) = g^{ij}\left(\nabla^2 u\right)_{ij}, \tag{1.11}$$

we can show

$$J\left(\omega(t,x)\right)^{1/2}\left(\frac{\det g(\omega(t,x))}{\det g(x)}\right)^{1/4} = \exp\left(\int_1^t \frac{1}{4s}\left(-\Delta r^2\right)\left(\omega(s,x)\right)\mathrm{d}s\right).$$

The right hand side of this identity is a geometric invariant, and indeed it shows in combination with the group property $\omega(t,\omega(s,x)) = \omega(ts,x)$ the formula (1.10). Note, as a consequence of (1.10), that $C_c^\infty(M)$ is left invariant under dilations (in particular the generator A is essentially self-adjoint on $C_c^\infty(M)$). We also note that ω fixes ∂O and, moreover,

$$\omega(t,x) = \exp|_{N^+\partial O}\left[\frac{1}{t}\left(\exp|_{N^+\partial O}\right)^{-1}(x)\right] \quad \text{for } (t,x) \in (0,\infty)\times E. \tag{1.12}$$

Hence $\mathrm{e}^{-\mathrm{i}\frac{\ln t}{2}A}$ is unitary on $\mathcal{H}_{\mathrm{aux}} := L^2(E) \subset \mathcal{H}$ and $(\mathcal{H}_{\mathrm{aux}})^\perp = L^2(O) \subset \mathcal{H}$, respectively. By (1.12) $\mathrm{e}^{-\mathrm{i}\frac{\ln t}{2}A}|_{\mathcal{H}_{\mathrm{aux}}}$ is the "geodesic dilation" on E (since the composition part is given in geodesic spherical coordinates by $r \to r/t$), while $\mathrm{e}^{-\mathrm{i}\frac{\ln t}{2}A}|_{(\mathcal{H}_{\mathrm{aux}})^{\perp}}$ does not have a similar geometric meaning. Moreover, due to the eikonal equation

$$|\operatorname{grad} r|_g^2 = g^{ij}(\partial_i r)(\partial_j r) = 1 \quad \text{on } E \tag{1.13}$$

it follows that K is a solution to the Hamilton–Jacobi equation

$$\partial_t K = -\frac{1}{2} g^{ij}(\partial_i K)(\partial_j K) \quad \text{on } E. \tag{1.14}$$

Theorem 1.5. *Let (M, g) be a connected complete Riemannian manifold satisfying Conditions 1.1–1.3, and V a potential satisfying Condition 1.4. Then, for the Schrödinger propagator $\mathrm{e}^{-\mathrm{i}tH}$ for (1.1) and the free propagator (1.8a) there exists the wave operator*

$$\Omega_+ = \text{s-}\lim_{t\to+\infty} \mathrm{e}^{\mathrm{i}tH} U(t) P_{\mathrm{aux}},$$

where P_{aux} is the projection onto $\mathcal{H}_{\mathrm{aux}}$. Moreover there exists the limit

$$\tilde{\Omega}_+ = \text{s-}\lim_{t\to+\infty} U(t)^* \mathrm{e}^{-\mathrm{i}tH} P_{\mathrm{c}},$$

where P_{c} is the projection onto the continuous subspace $\mathcal{H}_{\mathrm{c}}(H) = \chi_{(0,\infty)}(H)\mathcal{H}$ for H.

Finally Ω_+ is complete, i.e.

$$\tilde{\Omega}_+ = \Omega_+^*, \qquad \Omega_+^*\Omega_+ = P_{\mathrm{aux}} \quad \textit{and} \quad \Omega_+\Omega_+^* = P_{\mathrm{c}}. \tag{1.15}$$

Here we used the notation $\chi_{\mathcal{O}}$ to denote the characteristic function of a subset $\mathcal{O} \subseteq \mathbb{R}$. Note that $U(t)P_{\mathrm{aux}}$ and Ω_+ are independent of the extension of r to O. The fact that H does not have positive eigenvalues is proved under weaker conditions in [16] and will not be discussed in this paper. It follows by a standard local compactness argument that the negative spectrum of H (if not empty) consists of finite multiplicity eigenvalues accumulating at most at zero.

Note that $t \cdot r(\omega(t, x)) = r(x)$ for $(t, x) \in (0, \infty) \times E$. By this formula it follows readily that

$$\Omega_+^* H \Omega_+ = M_f P_{\mathrm{aux}}; \quad f = 2^{-1} r(\cdot)^2. \tag{1.16}$$

Here M_f means the operator given by multiplication by f (defined maximally on $\mathcal{H}$). Consequently we immediately deduce

Corollary 1.6 *(Spectrum). The continuous spectrum $\sigma_{\mathrm{c}}(H) = \sigma(H_{\mathrm{c}}) = [0, \infty)$ and the singular continuous spectrum of H is absent* (*i.e.* $\sigma_{\mathrm{sc}}(H) = \emptyset$).

Note that under Conditions 1.1 and 1.3 the essential spectrum $\sigma_{\mathrm{ess}}(H_0) = [0, \infty)$, see [18, Theorem 1.2]. On the other hand the second part of the corollary on the singular continuous spectrum of H is new.

As another corollary, the existence of "the asymptotic speed" follows (see for example [6] for notation).

Corollary 1.7 *(Asymptotic observables). In the space $\mathcal{H}_c(H)$ there exists the $*$-representation*

$$\omega_\infty^+ = \mathrm{s} - C_c(M) - \lim_{t\to+\infty} \mathrm{e}^{\mathrm{i}tH}\omega(t,\cdot)\mathrm{e}^{-\mathrm{i}tH}.$$

In particular the asymptotic speed

$$r\big(\omega_\infty^+\big) = \mathrm{s} - C_c(\mathbb{R}) - \lim_{t\to+\infty} \mathrm{e}^{\mathrm{i}tH}\frac{r(\cdot)}{t}\mathrm{e}^{-\mathrm{i}tH}$$

exists as a self-adjoint operator on $\mathcal{H}_c(H)$. This operator is positive with zero kernel.

Moreover, for all $\phi \in C_c(M)$

$$\phi\big(\omega_\infty^+\big) = \Omega_+ M_\phi \Omega_+^* \quad \textit{and} \quad H_c = 2^{-1} r\big(\omega_\infty^+\big)^2. \tag{1.17}$$

Remarks 1.8.

1) A principal virtue of the formula (1.8a) is its intrinsic "position space" nature. In Euclidean scattering such formula appeared first in [27]; for later developments see [7,14,3]. It was conceived in [4] for a general geometric setting. Another virtue of (1.8a) is that time reversal invariance applies yielding existence and completeness of a similar wave operator Ω_- (constructed by taking $t \to -\infty$). Whence Theorem 1.5 defines a scattering theory that includes a unitary scattering operator, however we shall not elaborate here.
2) We note that Conditions 1.2–1.4 in some sense are optimal, see Subsection 2.2 for counter examples to Theorem 1.5 under the slight relaxation of conditions given by allowing either $\delta = 0$ in (1.3), $\kappa = 0$ in (1.6a) or $\eta = 0$ in (1.7).
3) If we denote the *time-dependent generator* of $U(t)$ by $G(t)$ then in the geodesic spherical coordinates

$$G(t) = \frac{1}{2}p_r^* p_r - \frac{1}{2}\left(p_r - \frac{r}{t}\right)^*\left(p_r - \frac{r}{t}\right) \quad \text{on } E;\ p_r := (\partial_k r) g^{kl} p_l.$$

By arguments motivated by Classical Mechanics the second term is *short-range*. In fact we also have that $G(t) = H_0 - W(t) - \alpha(t)$ where

$$W(t) := \frac{1}{2}(p_i - \partial_i K)^* g^{ij}(p_j - \partial_j K) \quad \text{and} \quad \alpha(t) := (\partial_t K) + \frac{1}{2}g^{ij}(\partial_i K)(\partial_j K),$$

and we prove in this paper, more generally, that $W(t)$ is short-range. This is in fact the heart of the proof of Theorem 1.5. Whence the generator of $U(t)$ differs from the one-dimensional radial Laplacian by a short-range term, see [15] for a similar relationship.
4) The subset O is not uniquely determined in Condition 1.1, but the wave operator is nevertheless (at least partially) in some sense unique. We will discuss this issue in Subsection 1.1. We show that there is an explicit dependence on the one-parameter family of sets $O_a \supseteq O$ induced by the outward geodesic flow ($\partial O_a = \{r = a\}$; $a \geqslant 0$). This idea is exploited in Subsection 1.2 where we introduce a stronger condition than Condition 1.1 (regularity of the geodesic flow from a point rather than from a submanifold). Our main results are easily implemented in this setting, although it is also possible (as an alternative way of showing results in this setting) to mimic the procedure in the bulk of the paper.

1.1. Uniqueness of the wave operator

Let us assume Conditions 1.1–1.4. We set for $a \geqslant 0$

$$O_a = \{x \in E;\ r(x) < a\} \cup \overline{O}, \qquad r_a(x) = r(x) - a,$$

and decorate various quantities defined previously with respect to O_a and r_a by the subscript a. In particular we discuss the strong limits

$$V_a = V_a^0 = \text{s-}\lim_{t\to+\infty} U(t)^* U_a(t) P_{\text{aux}}^{(a)},$$
$$V^a = V_0^a = \text{s-}\lim_{t\to+\infty} U_a(t)^* U(t) P_{\text{aux}}.$$

For $u \in \mathcal{H}$

$$U_a(t)u(x) = \mathrm{e}^{\mathrm{i}r_a(x)^2/2t}\left(\det \frac{\partial \omega_a(t,x)}{\partial x}\right)^{1/2}\left(\frac{\det g(\omega_a(t,x))}{\det g(x)}\right)^{1/4} u\bigl(\omega_a(t,x)\bigr)$$

and since $\omega(t,\cdot)^{-1}(x) = \omega(1/t,x)$

$$U_a(t)^* u(x) = \mathrm{e}^{-\mathrm{i}t r_a(x)^2/2}\left(\det \frac{\partial \omega_a(1/t,x)}{\partial x}\right)^{1/2}\left(\frac{\det g(\omega_a(1/t,x))}{\det g(x)}\right)^{1/4} u\bigl(\omega_a(1/t,x)\bigr).$$

We note that the flow ω_a satisfies

$$r_a\bigl(\omega_a(t,x)\bigr) = r_a(x)/t \quad \text{for } x \in E_a. \tag{1.18}$$

Let $u \in \mathcal{H}$. Then for $x \in O_{a/t}$

$$U(t)^* U_a(t) P_{\text{aux}}^{(a)} u(x) = 0,$$

and for $x \in E_{a/t}$

$$\begin{aligned}
&U(t)^* U_a(t) P_{\text{aux}}^{(a)} u(x)\\
&\quad = \mathrm{e}^{\mathrm{i}r_a(\omega(1/t,x))^2/2t - \mathrm{i}t r(x)^2/2}\left(\det \frac{\partial \omega_a(t,\cdot)}{\partial x}\bigl(\omega(1/t,x)\bigr)\right)^{1/2}\left(\det \frac{\partial \omega(1/t,x)}{\partial x}\right)^{1/2}\\
&\qquad \times \left(\frac{\det g(\omega_a(t,\omega(1/t,x)))}{\det g(\omega(1/t,x))}\right)^{1/4}\left(\frac{\det g(\omega(1/t,x))}{\det g(x)}\right)^{1/4} u\bigl(\omega_a\bigl(t,\omega(1/t,x)\bigr)\bigr)\\
&\quad = \mathrm{e}^{-\mathrm{i}ar(x) + \mathrm{i}a^2/2t}\left(\det \frac{\partial \tau_{a(1-1/t)}(x)}{\partial x}\right)^{1/2}\left(\frac{\det g(\tau_{a(1-1/t)}(x))}{\det g(x)}\right)^{1/4} u\bigl(\tau_{a(1-1/t)}(x)\bigr),
\end{aligned}$$

where for the first factor we have used by (1.18)

$$r_a\bigl(\omega(1/t,x)\bigr) = r\bigl(\omega(1/t,x)\bigr) - a = tr(x) - a,$$

and for the others we have set

$$\omega_a\big(t, \omega(1/t, x)\big) = \tau_{a(1-1/t)}(x).$$

In fact τ_b is radial translation given in spherical coordinates by $\tau_b x(r,\sigma) = x(r+b,\sigma)$ for $r > \max(0, -b)$. Note $r(\omega(1/t, x)) = tr$, so that

$$r_a\big(\omega_a\big(t, \omega(1/t, x)\big)\big) = (tr - a)/t = r_a + a(1 - 1/t).$$

Hence the limit V_a exists, $\operatorname{Ran} V_a \subseteq \mathcal{H}_{\mathrm{aux}}$ and for $x \in E$

$$V_a u(x) = \mathrm{e}^{-\mathrm{i}ar(x)}\left(\det \frac{\partial \tau_a(x)}{\partial x}\right)^{1/2}\left(\frac{\det g(\tau_a(x))}{\det g(x)}\right)^{1/4} u\big(\tau_a(x)\big). \tag{1.19}$$

Using (1.19) we see that in fact V_a is a unitary map $\mathcal{H}^{(a)}_{\mathrm{aux}} \to \mathcal{H}_{\mathrm{aux}}$. From this unitarity property it follows that also the limit V^a exists, that V^a is a unitary map $\mathcal{H}_{\mathrm{aux}} \to \mathcal{H}^{(a)}_{\mathrm{aux}}$ and that $V^a = V_a^*$.

Thus we have the following relationship between the wave operators Ω_a and Ω_b:

$$\Omega_a = \Omega_b V_a^b; \quad V_a^b := V^b V_a. \tag{1.20}$$

In fact, more generally, the existence of Ω_b implies the existence of Ω_a and (1.20) is then valid (here we use that the limits V^b and V_a exist and the intertwining rule for wave operators).

1.2. Manifold with a pole

Let us consider an "extreme case" of the previous setting. We assume, instead of Condition 1.1:

Condition 1.9. The manifold M has a *pole* o, that is, there exists a point $o \in M$ such that the exponential map: $\exp_o : TM_o \to M$ is diffeomorphic.

Note Condition 1.9 is indeed stronger than Condition 1.1, because under Condition 1.9 we can choose any geodesic ball for O.

We consider the distance function $r(x) = \operatorname{dist}(x, o)$. It is not smooth at o, but r^2 is. Hence Condition 1.2 makes sense with $r_0 = 0$ for the function r^2. Throughout this subsection, when we refer to Condition 1.2 we mean Condition 1.2 with $r_0 = 0$.

Define the free propagator $U(t)$, $t > 0$, by

$$U(t) = \mathrm{e}^{\mathrm{i}K(t,\cdot)}\mathrm{e}^{-\mathrm{i}\frac{\ln t}{2}A}$$

with K and A given by (1.8b) and (1.8c), respectively, in terms of the above r^2. Then $\mathrm{e}^{-\mathrm{i}\frac{\ln t}{2}A}$ is the geodesic dilation with respect to o, and we have the formula

$$U(t)u(x) = \mathrm{e}^{\mathrm{i}r(x)^2/2t}\exp\left(\int_1^t \frac{1}{4s}\big(-\Delta r^2\big)\big(\omega(s,x)\big)\,\mathrm{d}s\right)u\big(\omega(t,x)\big),$$

where

$$\omega(t,x) = \exp_o\left[\frac{1}{t}(\exp_o)^{-1}(x)\right] \quad \text{for } (t,x) \in (0,\infty) \times M.$$

Theorem 1.10. *Suppose Conditions 1.9 and 1.2–1.4. Then there exist the strong limits*

$$\Omega_+ = \mathrm{s-}\lim_{t\to+\infty} \mathrm{e}^{\mathrm{i}tH} U(t) \quad \textit{and} \quad \tilde{\Omega}_+ = \mathrm{s-}\lim_{t\to+\infty} U(t)^* \mathrm{e}^{-\mathrm{i}tH} P_{\mathrm{c}},$$

where P_{c} is the projection onto $\mathcal{H}_{\mathrm{c}}(H) = \chi_{(0,\infty)}(H)\mathcal{H}$, and the wave operator Ω_+ is complete, i.e.

$$\tilde{\Omega}_+ = \Omega_+^*, \qquad \Omega_+^*\Omega_+ = I \quad \textit{and} \quad \Omega_+\Omega_+^* = P_{\mathrm{c}}.$$

The result follows by combining Theorem 1.5 and Subsection 1.1. In fact the arguments in Subsection 1.1 extend and are valid including the "degenerate" situation $O = \{o\}$ (even though this set is not open).

Finally we write down the corresponding corollaries: Noting

$$\Omega_+^* H \Omega_+ = M_f; \quad f = 2^{-1} r(\cdot)^2,$$

we have

Corollary 1.11 *(Spectrum). The singular continuous spectrum of H is absent, i.e. $\sigma_{\mathrm{sc}}(H) = \emptyset$, and the continuous spectrum $\sigma_{\mathrm{c}}(H) = \sigma(H_{\mathrm{c}}) = [0,\infty)$.*

Corollary 1.12 *(Asymptotic observables). In the space $\mathcal{H}_{\mathrm{c}}(H)$ there exists the $*$-representation*

$$\omega_\infty^+ = \mathrm{s} - C_{\mathrm{c}}(M) - \lim_{t\to+\infty} \mathrm{e}^{\mathrm{i}tH} \omega(t,\cdot) \mathrm{e}^{-\mathrm{i}tH}.$$

In particular the asymptotic speed

$$r\big(\omega_\infty^+\big) = \mathrm{s} - C_{\mathrm{c}}(\mathbb{R}) - \lim_{t\to+\infty} \mathrm{e}^{\mathrm{i}tH} \frac{r(\cdot)}{t} \mathrm{e}^{-\mathrm{i}tH}$$

exists as a self-adjoint operator on $\mathcal{H}_{\mathrm{c}}(H)$. This operator is positive with zero kernel.

Moreover, for all $\phi \in C_{\mathrm{c}}(M)$

$$\phi\big(\omega_\infty^+\big) = \Omega_+ M_\phi \Omega_+^* \quad \textit{and} \quad H_{\mathrm{c}} = 2^{-1} r\big(\omega_\infty^+\big)^2.$$

Remark 1.13. Under Condition 1.9 a sufficient condition for Condition 1.2 is the following: Suppose there exists $\delta \in (0,1)$ such that the radial curvature $R = R(\dot{x},\cdot,\dot{x},\cdot)$ satisfies the upper bound

$$R \leqslant \frac{1-\delta^2}{4r^2} g. \tag{1.21}$$

This is along any unit-speed geodesic $x(\cdot)$ emanating from the pole o of Condition 1.9 and with $r = r(x)$. (Alternatively $R_{ij} = (\nabla r)_k (\nabla r)^l R^k{}_{ilj}$ in terms of the curvature tensor as defined in [17,22].)

Then by a standard comparison argument, see for example [13, Proof of Theorem 4.1.1], indeed (1.4) holds true with this δ. In particular if M has non-positive sectional curvatures (1.4) is valid for $\delta = 1$. For these considerations Condition 1.3 is irrelevant. Note that (1.21) involves second order derivatives of the metric. In some principal examples, see Subsubsection 2.1.3, we shall use a different criterion involving derivatives of the metric up to first order only.

2. Geometric setting considerations

We shall explore the generality and limitations of our conditions in terms of various examples. The fact that these conditions are invariant under change of variables will facilitate the construction of examples. Secondly we shall explore the consequences of our conditions in Classical Mechanics.

2.1. Examples

We give various examples. For convenience we assume Condition 1.9 instead of Condition 1.1, and take henceforth $r_0 = 0$ in Condition 1.2 and $V = 0$ in Condition 1.4.

2.1.1. Warped product manifold

Under Condition 1.9 we can write

$$g = \mathrm{d}r \otimes \mathrm{d}r + g_{\alpha\beta}(r,\sigma)\,\mathrm{d}\sigma^\alpha \otimes \mathrm{d}\sigma^\beta; \qquad g_{rr} = 1, \qquad g_{r\alpha} = g_{\alpha r} = 0,$$

where σ^α are local coordinates on the geodesic unit sphere S_1 and the Greek indices run on $2, \dots, d$. A *warped product manifold* is a connected complete Riemannian manifold fulfilling Condition 1.9 with a Riemannian metric of the form

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

in the geodesic spherical coordinates. Note that this in particular means (due to a regularity consideration at the pole o) that h is the standard Euclidean metric density of the unit sphere and that $\lim_{r\to 0} r^{-2} f(r) = 1$. In the framework of Condition 1.1 such restriction on h is not needed.

Let us assume (M^d, g) is a warped product manifold. Then, if we set $f = \mathrm{e}^{2\varphi}$, (1.3) is equivalent to

$$2r\varphi' \geqslant 1 + \delta, \tag{2.1}$$

and (1.6a) to

$$\bigl|(r\varphi')'\bigr| \leqslant C\langle r\rangle^{-1/2-\kappa}. \tag{2.2}$$

In fact, by direct computations,

$$(\nabla^2 r^2)_{rr} = 2, \qquad (\nabla^2 r^2)_{r\alpha} = (\nabla^2 r^2)_{\alpha r} = 0, \qquad (\nabla^2 r^2)_{\alpha\beta} = r f' h_{\alpha\beta}. \tag{2.3}$$

Clearly the lower bound (2.1) results from (2.3). Similarly the bound (2.2) results by taking the trace of (2.3), cf. (1.11), to obtain that $\Delta r^2 = 2 + 2(d-1)r\varphi'$, and then noting that this quantity is radially symmetric.

We see that the inequalities (2.1) and (2.2) allow, for example,

$$f_{1,\mu}(r) = r^2\langle r\rangle^{2\mu}, \quad \mu \geqslant (\delta-1)/2, \qquad f_{2,\nu}(r) = r^2 \mathrm{e}^{-2}\exp\bigl(2\langle r\rangle^{\nu}\bigr), \quad 0 \leqslant \nu \leqslant 1/2-\kappa.$$

The Euclidean space corresponds to $f_{1,0}(r) = f_{2,0}(r) = r^2$.

2.1.2. Ultra-long-range perturbation of Euclidean space

Though we have formulated our conditions in a coordinate invariant way, our first motivation was the example $M = \mathbb{R}^d$ with a Riemannian metric g satisfying Conditions 1.9, 1.2 and

Condition 2.1. There exists $c > 0$ such that for the standard coordinates x

$$g \geqslant c\delta_{ij}\,\mathrm{d}x^i \otimes \mathrm{d}x^j$$

and that for $r = \mathrm{dist}_g(x, 0)$

$$\bigl|\partial_x^\alpha g_{ij}\bigr| \leqslant C_\alpha \langle x\rangle^{-|\alpha|} \quad \text{for } |\alpha| \leqslant 2,$$
$$\bigl|\partial_x^\alpha \bigl(\nabla^2 r^2\bigr)_{ij}\bigr| \leqslant C_\alpha \langle x\rangle^{-|\alpha|} \quad \text{for } |\alpha| \leqslant 1.$$

Condition 2.1 is stronger than Condition 1.3. Note also that Condition 2.1 is manifestly not coordinate invariant requiring g to be comparable with the Euclidean metric.

An example of a model satisfying Conditions 1.9, 1.2 and 2.1 is given as follows: Let m be a real symmetric $d \times d$-matrix-valued function on $\mathbb{R}^d$. Suppose in addition that all entries $m_{ij} \in C^\infty(\mathbb{R}^d)$ and obey

$$\bigl|\partial_x^\alpha m_{ij}\bigr| \leqslant C_\alpha \langle x\rangle^{-|\alpha|} \quad \text{for } |\alpha| \leqslant 3. \tag{2.4}$$

Then for any $\epsilon \in \mathbb{R}$ with $|\epsilon|$ being sufficiently small the metric g given as a matrix by $g_{ij} = \delta_{ij} + \epsilon m_{ij}$ fulfills Conditions 1.9, 1.2 and 2.1. We refer to [5] for details.

In fact there is a more general example from [5]: Take any "unperturbed" metric g on $\mathbb{R}^d$ obeying

$$g \geqslant c\delta_{ij}\,\mathrm{d}x^i \otimes \mathrm{d}x^j, \qquad \bigl|\partial_x^\alpha g_{ij}\bigr| \leqslant C_\alpha \langle x\rangle^{-|\alpha|} \quad \text{for } |\alpha| \leqslant 3 \tag{2.5}$$

and identified in terms of the Euclidean metric on $\mathbb{R}^d$ as a matrix of the form (for $x \neq 0$)

$$G(x) = P + P_\perp G(x) P_\perp, \tag{2.6}$$

where P denotes, in the Dirac notation, the orthogonal projection $P = P(\hat{x}) = |\hat{x}\rangle\langle\hat{x}|$ parallel to $\hat{x} = x/|x|$ and $P_\perp = P_\perp(\hat{x}) = I - P$ the orthogonal projection onto $\{\hat{x}\}^\perp$. Suppose in addition that

$$P_\perp\bigl((1-\delta)G(x) + x\cdot\nabla G(x)\bigr)P_\perp \geqslant 0. \tag{2.7}$$

Then a computation shows that the conditions of [5, Theorem 1.4 ii)] as well as Condition 1.2 (with this δ in Condition 1.2 and with $\bar{c} := (1+\delta)/2$ in [5, (1.13)]) are fulfilled. In fact using (2.6) we compute

$$\nabla^2 r^2(x)(y,y) = 2yG(x)y + yP_\perp \nabla G(x) \cdot xP_\perp y,$$

showing the equivalence of Condition 1.2 and (2.7) for a metric of the form (2.6). (Note at this point the consistency with (2.1).)

If we again let m be given by (2.4) and similarly define $(g_\epsilon)_{ij} = g_{ij} + \epsilon m_{ij}$ then a computation using [5, Theorems 1.4 ii) and 1.6] shows that indeed g_ϵ for any sufficiently small $|\epsilon|$ fulfills Conditions 1.9, 1.2 and 2.1. For some examples constructed in this way we refer to Subsubsection 2.1.3. As the reader will see the geometric invariance is exploited explicitly.

2.1.3. *Conformally flat manifold*

The Laplace–Beltrami operator, the comparison dynamics (1.8a) and Conditions 1.1–1.3 (as well as Condition 1.4) are cleanly geometrically invariant, while Condition 2.1 is not that appealing. One way to circumvent this for given (M, g_M), M being connected, complete and d-dimensional, is by postulating the existence of a diffeomorphism $\Psi : M \to \mathbb{R}^d$ with the property that

$$g := (\Psi^*)^{-1} g_M \quad \text{obeys Condition 2.1.} \tag{2.8}$$

Clearly Conditions 1.9, 1.2 and (2.8) constitutes an invariant theory.

We will in this subsubsection give an example of the how to use (2.8) concretely. Our discussion is based on [5, Section 7]. Consider a radial function $V = V(z) = V(|z|)$ of class C^∞ on $\mathbb{R}^d$, $d \geqslant 2$, for which there are constants $\mu \in (-\infty, 2)$, $a, A, \sigma > 0$ and $\delta \in (0,1]$ such that

$$-A\langle z\rangle^{-\mu} \leqslant V(z) \leqslant -a\langle z\rangle^{-\mu}, \tag{2.9a}$$

$$z \cdot \nabla V(z) + 2V(z) \leqslant \sigma V(z), \tag{2.9b}$$

$$\partial^\alpha V(z) = O\big(\langle z\rangle^{-(\mu+|\alpha|)}\big) \quad \text{for } |\alpha| \leqslant 3, \tag{2.9c}$$

$$(1+\delta) \leqslant \inf_{r>0} h(r); \qquad h(r) := \frac{(2 + \frac{-rV'(r)}{-V(r)}) \int_0^r \sqrt{-V(s)}\,\mathrm{d}s}{\sqrt{-V(r)}r}. \tag{2.9d}$$

Note that for any $\mu \in [0,1)$ obviously the function $V(z) = -\langle z\rangle^{-\mu}$ is an example in this class. A more careful (but elementary) consideration shows that this is the case for any $\mu \in (-\infty, 4/3)$. It could be true for any $\mu \in (-\infty, 2)$ (note that $h(0) = h(\infty) = 2$). If $W = W(z)$ is of class C^∞ on $\mathbb{R}^d$, possibly non-radial, we are interested in studying the metric (conformally) generated by $V_\epsilon = V + \epsilon W$ for $|\epsilon| \geqslant 0$ sufficiently small, that is the metric

$$-2V_\epsilon\,\mathrm{d}z^2. \tag{2.10}$$

We shall impose a condition on W similar to (2.9c),

$$\partial^\alpha W(z) = O\big(\langle z\rangle^{-(\mu+|\alpha|)}\big) \quad \text{for } |\alpha| \leqslant 3. \tag{2.11}$$

Under the conditions (2.9a)–(2.9c) and (2.11) a diffeomorphism Ψ as in (2.8) is constructed in [5, Subsections 7.1–7.2] so that in the new coordinates in fact Conditions 1.9 and 2.1 (and therefore Conditions 1.9 and 1.3) are fulfilled. The new condition (2.9d) is introduced, as we will show below, to verify the remaining Condition 1.2 (in our discussion the potential in (1.1) is for simplicity taken absent). Following [5] we define Ψ by specifying its inverse,

$$\Psi^{-1}(x) = \exp_0\bigl(x/\bigl(-2V(0)\bigr)\bigr), \tag{2.12}$$

where the exponential mapping is defined in terms of the unperturbed metric, i.e. by (2.10) with $\epsilon = 0$. Concretely

$$x = \Psi(z) = \rho\bigl(|z|\bigr)\frac{z}{|z|} \quad \text{where } \rho(r) = \int_0^r \sqrt{-2V(s)}\,\mathrm{d}s. \tag{2.13}$$

Letting $r = r(\rho)$ denote the inverse of this function ρ we define

$$f(\rho) = \frac{\sqrt{-2V(r(\rho))}r(\rho)}{\rho}, \tag{2.14}$$

and we have

$$g_\epsilon := \bigl(\Psi^*\bigr)^{-1}\bigl(-2V_\epsilon\,\mathrm{d}^2z\bigr) = P + f^2P_\perp + O(\epsilon), \tag{2.15}$$

where P and $P_\perp$ are given as in (2.6). It remains (for Condition 1.2) to show that indeed (2.7) holds for the unperturbed part, $G := P + f^2P_\perp$, given the condition (2.9d): We compute

$$\rho\frac{\mathrm{d}}{\mathrm{d}\rho}f^2 + (1-\delta)f^2 = f^2\biggl(\biggl(2 + \frac{-rV'(r)}{-V(r)}\biggr)/f - 1 - \delta\biggr) = f^2\bigl(h(r) - 1 - \delta\bigr);$$

whence indeed by (2.9d)

$$P_\perp\bigl((1-\delta)G(x) + x\cdot\nabla G(x)\bigr)P_\perp \geqslant 0,$$

and therefore Condition 1.2 holds for the metrics g_ϵ and $-2V_\epsilon\,\mathrm{d}z^2$ for any slightly smaller $\delta > 0$ provided $|\epsilon| \geqslant 0$ is taken small enough. In particular our results apply to the metric $-2V_\epsilon\,\mathrm{d}z^2$ although this example from the outset does not conform with Condition 2.1 (unless $\mu = 0$).

We refer the reader to [5, Subsection 7.3] for an example with $\mu = 0$ in the previous scheme for which the geodesics of the perturbed metric emanating from $0 \in \mathbb{R}^d$ are attracted to logarithmic spirals.

2.2. *Counter examples, borderlines of conditions*

We construct warped product manifolds to illustrate the optimality of the conditions of Theorem 1.5.

Proposition 2.2. *Suppose Condition 1.9. Suppose that exactly one of the conditions $\delta > 0$, $\kappa > 0$ and $\eta > 0$ in Conditions 1.2–1.4 is replaced by either $\delta = 0$, $\kappa = 0$ or $\eta = 0$, respectively. Then the exists a warped product manifold fulfilling this slightly more general set of conditions for which not all of the analogous conclusions of Theorem 1.5 are true.*

In the case of $\delta = 0$ we can choose the density factor $f(r) = r^2\langle r\rangle^{-1}$ in Subsubsection 2.1.1. In the case of $\kappa = 0$ we can choose the density factor $f(r) = r^2 e^{-2} e^{2\sqrt{\langle r\rangle}}$. While for $\eta = 0$ we can choose the density factor $f(r) = r^2$ (Euclidean model) and $V = c\langle r\rangle^{-1}$, $c \neq 0$.

To see this we need some preparation. We introduce the Hilbert space $\tilde{\mathcal{H}} = L^2(\mathbb{R}_+, \mathcal{G}, dr)$ where $\mathcal{G} = L^2(S_1, d\sigma)$ where S_1 is the unit sphere in $\mathbb{R}^d$ and $d\sigma$ the induced Euclidean measure. For any warped product model $f = e^{2\phi}$ we introduce a unitary operator $\mathcal{M} : \mathcal{H} \to \tilde{\mathcal{H}}$ by

$$\tilde{u} = \mathcal{M}u = f(r)^{\frac{d-1}{4}} u = f(1)^{\frac{d-1}{4}} e^{\int_1^r \Delta r\, dr/2} u.$$

We have the formula in spherical coordinates (r, σ)

$$\tilde{U}(t)\tilde{u} := \mathcal{M}U(t)\mathcal{M}^{-1}\tilde{u} = e^{i\frac{r^2}{2t}} t^{-1/2}\tilde{u}\left(\frac{r}{t}, \sigma\right).$$

Note also the formula

$$\tilde{H}\tilde{u} := \mathcal{M}H\mathcal{M}^{-1}\tilde{u} = \left(\frac{1}{2}p_r^2 + \tilde{V} - \frac{1}{2}f^{-1}\Delta_1\right)\tilde{u},$$

where

$$p_r = -i\frac{d}{dr}, \qquad \tilde{V} = V + \frac{1}{8}(\Delta r)^2 + \frac{1}{4}\partial\Delta r,$$

and Δ_1 denotes the Laplace–Beltrami operator on $\mathcal{G}$.

The generator of $\tilde{U}(t)$ is given by

$$\tilde{G}(t) = \frac{1}{2}p_r^2 - \frac{1}{2}\left(p_r - \frac{r}{t}\right)^2,$$

cf. Remark 1.8 3). Whence we have for all $\tilde{u} \in C_c^\infty(\mathbb{R}_+ \times S_1)$

$$\big(\tilde{H} - \tilde{G}(t)\big)\tilde{U}(t)\tilde{u} = t^{-1/2} e^{i\frac{r^2}{2t}}\left(-\frac{1}{2}p_r^2 + \tilde{V} - \frac{1}{2}f^{-1}\Delta_1\right)\tilde{u}\left(\frac{r}{t}, \sigma\right).$$

Given Conditions 1.2–1.4 for the model, and therefore (1.6b), (2.1) and (2.2), the Cook method and this computation yields the existence of the limit

$$\tilde{\Omega}\tilde{u} = \lim_{t\to\infty} e^{i\tilde{H}t}\tilde{U}(t)\tilde{u}; \quad \tilde{u} \in \tilde{\mathcal{H}}. \tag{2.16}$$

Moreover this argument does not work if $\delta = 0$ in Condition 1.2 (since then f^{-1} might not decay fast enough), or if $\kappa = 0$ in Condition 1.3 (since then $(\Delta r)^2$ might not decay fast enough) nor if

$\eta = 0$ in Condition 1.4 (since then V might not decay fast enough). This provides some intuition about Proposition 2.2.

To come closer to a proof of Proposition 2.2 let us note that these borderline cases can be "repaired" by modified evolutions in the spirit of the Dollard evolution for Schrödinger operators. Thus, for the example $f(r) = r^2\langle r\rangle^{-1}$ the factor $f^{-1} \approx r^{-1}$, and if we take $\tilde{u} = v(r)Y_l(\sigma)$ for a spherical harmonic Y_l we have

$$-\frac{1}{2}f^{-1}\Delta_1\tilde{u}\left(\frac{r}{t},\cdot\right) \approx cr^{-1}\tilde{u}\left(\frac{r}{t},\cdot\right); \quad c = c(l) = -\frac{1}{2}(l + d/2 - 1).$$

This motivates us to introduce

$$\tilde{U}_l(t)\tilde{u} := \mathrm{e}^{\mathrm{i}(\frac{r^2}{2t} - c\frac{t}{\langle r\rangle}\ln\langle r\rangle)}t^{-1/2}\tilde{u}\left(\frac{r}{t},\sigma\right),$$

whose generator is

$$\tilde{G}_l(t) = \frac{1}{2}p_r^2 - \frac{1}{2}\left(p_r - \frac{r}{t}\right)^2 + c\frac{\ln\langle r\rangle}{\langle r\rangle^3} + c\frac{r^2}{\langle r\rangle^3}.$$

Note that $c\frac{r^2}{\langle r\rangle^3} \approx cr^{-1}$. Whence, by the arguments above for this example, we obtain the existence of the limit

$$\tilde{\Omega}_l\tilde{u} = \lim_{t\to\infty} \mathrm{e}^{\mathrm{i}\tilde{H}t}\tilde{U}_l(t)\tilde{u}; \quad \tilde{u} \in \tilde{\mathcal{H}}_l := L^2(\mathbb{R}_+) \otimes Y_l. \tag{2.17}$$

We note the property

$$\tilde{\Omega}_l^*\tilde{H}\tilde{\Omega}_l = M_\lambda,$$

where M_λ denotes multiplication by the function $r \to r^2/2$, $v(r) \otimes Y_l \to \frac{r^2}{2}v(r) \otimes Y_l$. (The reader may at this point consult the proof of (3.3).) In particular $\operatorname{Ran} \mathcal{M}^{-1}\tilde{\Omega}_l \subseteq \mathcal{H}_c(H)$.

Proof of Proposition 2.2. First we continue our discussion of the example $f(r) = r^2\langle r\rangle^{-1}$ for which $\delta = 0$. Suppose on the contrary that the conclusions of Theorem 1.5 are all true for this example. Let Ω_+ be given accordingly and $\tilde{\Omega}_l$ be given by (2.17). We derive a contradiction by taking an arbitrary nonzero $\tilde{v} \in L^2(\mathbb{R}_+)$, define $\tilde{u} = \tilde{v} \otimes Y_l$ with any l for which $c = c(l) \neq 0$ and compute

$$\begin{aligned}\Omega_+^*\mathcal{M}^{-1}\tilde{\Omega}_l\tilde{u} &= \Omega_+^*P_c\mathcal{M}^{-1}\tilde{\Omega}_l\tilde{u} = \lim_{t\to\infty} U(t)^*\mathcal{M}^{-1}\tilde{U}_l(t)\tilde{u} \\ &= \mathcal{M}^{-1}\lim_{t\to\infty}\left(\mathrm{e}^{-\mathrm{i}\frac{c}{r}\ln t}\tilde{w}\right) \otimes Y_l; \qquad \tilde{w}(r) = \mathrm{e}^{-\mathrm{i}\frac{c}{r}\ln r}\tilde{v}(r).\end{aligned}$$

Since $\tilde{w} \neq 0$ and $c \neq 0$ the factor $\mathrm{e}^{-\mathrm{i}\frac{c}{r}\ln t}$ does not have a limit when applied to $\tilde{w}$, cf. the Riemann–Lebesgue lemma [25]. This is a contradiction.

For the example $f(r) = r^2\mathrm{e}^{-2}\mathrm{e}^{2\sqrt{\langle r\rangle}}$, for which $\kappa = 0$, we proceed similarly. The term $\frac{1}{8}(\Delta r)^2 \approx cr^{-1}$, so we can repeat the above arguments.

Finally the potential $V = c\langle r\rangle^{-1}$, for which $\eta = 0$, provides (with $f = r^2$) a counter example. The arguments are the same. □

2.3. Classical Mechanics under Conditions 1.9 and 1.2

We outline proofs of analogues of Theorem 1.10 and Corollary 1.12 in Classical Mechanics. As we pointed out before the Classical Mechanics considerations only require Conditions 1.1 and 1.2. But, for convenience, we consider Conditions 1.9 and 1.2 with $r_0 = 0$, instead. If we adopt Conditions 1.1 and 1.2 not necessarily with $r_0 = 0$, then all the geodesics appearing below need to be non-trapped. Our proofs of Theorem 1.5 and Corollary 1.7 are strongly motivated by these considerations.

2.3.1. Regularity of classical dilation

First we prove an estimate for the geodesic dilation $\omega(t,x)$. Recall

$$\omega(t,x) = \exp_o\left[\frac{1}{t}\exp_o^{-1}(x)\right], \quad (t,x) \in (0,\infty) \times M.$$

In any local coordinates ω satisfies, cf. (1.9),

$$\partial_t \omega^i = -\frac{r}{t^2}(\operatorname{grad} r)(\omega) = -\frac{1}{2t} g^{ij}(\omega)\big(\partial_j r^2\big)(\omega), \qquad \omega(1,x) = x. \tag{2.18}$$

Lemma 2.3. *For all $(t,x) \in (0,\infty) \times M$ and independently of choice of coordinates*

$$g^{ij}(x) g_{kl}\big(\omega(t,x)\big)\big[\partial_i \omega^k(t,x)\big]\big[\partial_j \omega^l(t,x)\big] \leqslant d t^{-(1+\delta)}. \tag{2.19}$$

Proof. The left hand side of (2.19) is indeed independent of coordinates. Fix $x \in M$ and choose coordinates such that $g_{ij}(x) = \delta_{ij}$. Consider the vector fields along $\{\omega(t,x)\}_{t\in\mathbb{R}}$ given by $\partial_i \omega^\bullet(t,x)$ and $\partial_j \omega^\bullet(t,x)$. Since the Levi-Civita connection ∇ is compatible with the metric,

$$\frac{\partial}{\partial t} g_{kl}(\omega)\big(\partial_i \omega^k\big)\big(\partial_j \omega^l\big) = \frac{\partial}{\partial t}\big\langle \partial_i \omega^\bullet, \partial_j \omega^\bullet\big\rangle = \big\langle \nabla_{\partial_t \omega} \partial_i \omega^\bullet, \partial_j \omega^\bullet\big\rangle + \big\langle \partial_i \omega^\bullet, \nabla_{\partial_t \omega} \partial_j \omega^\bullet\big\rangle.$$

(The definition of $\nabla_{\partial_t \omega}$ is given below.) From (2.18) it follows that

$$\begin{aligned}
\nabla_{\partial_t \omega} \partial_i \omega^\bullet &= \partial_t \partial_i \omega^\bullet + \big(\partial_t \omega^k\big) \Gamma^\bullet_{kl} \partial_i \omega^l \\
&= -\frac{1}{2t}\big(\partial_i \omega^k\big)\partial_k\big(g^{\bullet l}\partial_l r^2\big) - \frac{1}{2t}\big(g^{km}\partial_m r^2\big)\Gamma^\bullet_{kl}\partial_i \omega^l \\
&= -\frac{1}{2t}\nabla_{\partial_i \omega}\big(g^{\bullet l}\partial_l r^2\big) = -\frac{1}{2t} g^{\bullet l}\big(\partial_i \omega^k\big)\big(\nabla^2 r^2\big)_{kl}.
\end{aligned}$$

Thus, taking summation in i, j, we obtain

$$\frac{\partial}{\partial t} g^{ij}(x) g_{kl}(\omega)\big(\partial_i \omega^k\big)\big(\partial_j \omega^l\big) \leqslant -\frac{1+\delta}{t} g^{ij}(x) g_{kl}(\omega)\big(\partial_i \omega^k\big)\big(\partial_j \omega^l\big).$$

Noting $g^{ij}(x) g_{kl}(\omega)(\partial_i \omega^k)(\partial_j \omega^l)|_{t=1} = d$, we have (2.19). □

2.3.2. Propagation estimates

Set

$$K(t,x)=\frac{r^2}{2t},\qquad h_0(x,\xi)=\frac{1}{2}g^{ij}\xi_i\xi_j,\qquad w(t,x,\xi)=\frac{1}{2}g^{ij}(\xi_i-\partial_i K)(\xi_j-\partial_j K)$$

for $t>0$, $x\in M$ and $(x,\xi)\in T^*M$.

Lemma 2.4. *For any Hamiltonian trajectory $(x(t),\xi(t))$ there exists $C>0$ such that*

$$w\big(t,x(t),\xi(t)\big)\leqslant Ct^{-(1+\delta)}. \tag{2.20}$$

Proof. We compute

$$\frac{\mathrm{d}}{\mathrm{d}t}w=\frac{\partial}{\partial t}w+\{h_0,w-h_0\}=\frac{\partial}{\partial t}w+\frac{\partial h}{\partial \xi}\frac{\partial}{\partial x}(w-h_0)-\frac{\partial h}{\partial x}\frac{\partial}{\partial \xi}(w-h_0).$$

By (1.14)

$$\frac{\partial}{\partial t}w=\frac{1}{2}g^{ij}\big(\partial_i g^{kl}(\partial_k K)(\partial_l K)\big)(\xi_j-\partial_j K).$$

Noting that by the compatibility condition $(\nabla g)^{ij}_k=0$, we have

$$0=\partial_k g^{ij}+\Gamma^i_{kl}g^{lj}+\Gamma^j_{kl}g^{il}, \tag{2.21}$$

so that

$$\partial_i g^{kl}(\partial_k K)(\partial_l K)=2\big(\nabla^2 K\big)_{ik}g^{kl}(\partial_l K). \tag{2.22}$$

Thus

$$\frac{\partial}{\partial t}w=(\partial_l K)g^{lk}\big(\nabla^2 K\big)_{ki}g^{ij}(\xi_j-\partial_j K).$$

On the other hand, by (2.21) and (2.22) again we have

$$\begin{aligned}
&\{h_0,w-h_0\}\\
&\quad=g^{ij}\xi_j\big[-\big(\partial_i g^{kl}\big)\xi_k(\partial_l K)-g^{kl}\xi_k(\partial_i\partial_l K)+\big(\nabla^2 K\big)_{ik}g^{kl}(\partial_l K)\big]+\frac{1}{2}\big(\partial_k g^{ij}\big)\xi_i\xi_j g^{kl}(\partial_l K)\\
&\quad=g^{ij}\xi_j\big(\Gamma^k_{im}g^{ml}+\Gamma^l_{im}g^{km}\big)\xi_k(\partial_l K)-g^{ij}\xi_j g^{kl}\xi_k(\partial_i\partial_l K)+g^{ij}\xi_j\big(\nabla^2 K\big)_{ik}g^{kl}(\partial_l K)\\
&\qquad-\frac{1}{2}\big(\Gamma^i_{km}g^{mj}+\Gamma^j_{km}g^{im}\big)\xi_i\xi_j g^{kl}(\partial_l K)\\
&\quad=g^{ij}\xi_j\Gamma^l_{im}g^{km}\xi_k(\partial_l K)-g^{ij}\xi_j g^{kl}\xi_k(\partial_i\partial_l K)+g^{ij}\xi_j\big(\nabla^2 K\big)_{ik}g^{kl}(\partial_l K)\\
&\quad=-\xi_j g^{ji}\big(\nabla^2 K\big)_{ik}g^{kl}(\xi_l-\partial_l K).
\end{aligned}$$

Hence, summing up and using Condition 1.2, we obtain

$$\frac{\mathrm{d}}{\mathrm{d}t} w = -(\xi_l - \partial_l K) g^{lk} \left(\nabla^2 K\right)_{ki} g^{ij} (\xi_j - \partial_j K) \leqslant -\frac{1+\delta}{t} w. \qquad \square$$

Proposition 2.5. *For any geodesic $x(t)$ there exists the limit*

$$\omega_\infty = \lim_{t\to\infty} \omega\big(t, x(t)\big). \tag{2.23}$$

Proof. Due to the flow equation (2.18) we have the group property $\omega(t, \omega(s, x)) = \omega(ts, x)$. Differentiate

$$\omega\big(t, \omega(s, x)\big) = \omega\big(s, \omega(t, x)\big)$$

in t, and use then (2.18) to obtain

$$\partial_t \omega^i \big(t, \omega(s, x)\big) = -\big(\partial_k \omega^i\big)\big(t, \omega(s, x)\big) g^{kl} \big(\omega(s, x)\big)(\partial_l K)\big(t, \omega(s, x)\big).$$

Putting $s = 1$, we obtain

$$\partial_t \omega^i (t, x) = -g^{kl}(x)\big(\partial_k \omega^i\big)(t, x)(\partial_l K)(t, x). \tag{2.24}$$

By applying first (2.24), and then (2.19) and (2.20), we obtain

$$\begin{aligned} g_{ij}\dot\omega^i\dot\omega^j &= g_{ij}\big[\partial_t\omega^i + (\partial_\xi h_0)\big(\partial_x\omega^i\big)\big]\big[\partial_t\omega^j + (\partial_\xi h_0)\big(\partial_x\omega^j\big)\big] \\ &= g_{ij} g^{kl}\big(\partial_k\omega^i\big)(\xi_l - \partial_l K) g^{mn}\big(\partial_m\omega^j\big)(\xi_n - \partial_n K) \\ &\leqslant C t^{-2(1+\delta)}, \end{aligned}$$

and the assertion follows. $\square$

2.3.3. Mourre estimate

We also note that the classical Mourre estimate holds. Since the geodesics equation is given by $\ddot x^i + \Gamma^i_{jk}\dot x^j \dot x^k = 0$, the following result is true.

Lemma 2.6. *For any geodesic $x(t)$ the following inequality holds*:

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2} r^2 \geqslant 2(1+\delta) h_0.$$

3. Reduction of the proof of Theorem 1.5

3.1. Reduction to existence of localization operators

Since we do not have enough regularities for the derivatives of g and $\nabla^2 r^2$, the Cook–Kuroda method does not apply even for the existence part of Theorem 1.5. We shall prove Theorem 1.5 in a symmetric manner for the existence and the completeness parts. In this subsection we reduce the proof to the construction of $Q_{\mathrm{f}}(t)$ and $Q_{\mathrm{p}}(t)$ which are time-dependent localization operators for the *free* and the *perturbed* dynamics, respectively.

We denote the time-dependent generator of $U(t)$ by $G(t)$, i.e.,

$$\frac{\mathrm{d}}{\mathrm{d}t}U(t) = -\mathrm{i}G(t)U(t).$$

It will not be important to known the domain of the generator but rather a convenient subspace. For that we observe that $U(t)$ and $U(t)^{-1}$ preserve the subspace $C_{\mathrm{c}}^{\infty}(M) \subseteq \mathcal{H}$, and hence $C_{\mathrm{c}}^{\infty}(M) \subseteq \mathcal{D}(G(t))$, and that the propagator acting on this subspace is explicitly given as follows (recall $H_0 = -\frac{1}{2}\Delta$):

$$G(t) = -\partial_t K + \mathrm{e}^{iK}\frac{1}{2t}A\mathrm{e}^{-iK} = H_0 - W(t) - \alpha(t); \tag{3.1a}$$

$$W(t) = \frac{1}{2}(p_i - \partial_i K)^* g^{ij}(p_j - \partial_j K) = \mathrm{e}^{\mathrm{i}K} H_0 \mathrm{e}^{-\mathrm{i}K}, \tag{3.1b}$$

$$\alpha(t) = \partial_t K + \frac{1}{2}g^{ij}(\partial_i K)(\partial_j K). \tag{3.1c}$$

Note by (1.14) that $\alpha(t) \equiv 0$ on E, and thus

$$\forall n \in \mathbb{N}\colon \quad |\alpha| = O\big(t^{-2}\langle r\rangle^{-n}\big) \quad \text{on } M. \tag{3.2}$$

For all practical purposes (in particular for stating Lemma 3.1 below) we can consider (3.1a) as a definition of a symmetric operator $G(t)$ on the domain $\mathcal{D}(H_0) \cap \mathcal{D}(H_0\mathrm{e}^{-\mathrm{i}K}) = \mathcal{D}(H_0) \cap \mathcal{D}(W(t))$.

As shown at the end of the subsection Theorem 1.5 is a consequence of the following two lemmas:

Lemma 3.1. *Let $0 < \mu < M < \infty$. Then there exists a weakly differentiable $Q_{\mathrm{f}} : [1, \infty) \to \mathcal{B}_{\mathrm{sa}}(\mathcal{H})$ such that $\|Q_{\mathrm{f}}(t)\|_{\mathcal{B}(\mathcal{H})} \leqslant 1$ and for some $\delta' > 0$*

i)

$$\mathrm{s-}\lim_{t\to\infty}\big(I - Q_{\mathrm{f}}(t)\big)U(t)\chi_{[\mu,M]}\big(r^2\big)P_{\mathrm{aux}} = 0,$$

where $\chi_{[\mu,M]}$ is the characteristic function for $[\mu, M]$ and $\chi_{[\mu,M]}(r^2)$ denotes the multiplier.

ii) *The operators $G(t)Q_f(t)$ and $Q_f(t)G(t)$ are bounded, and the Heisenberg derivative of $Q_f(t)$ with respect to $G(t)$ is non-negative modulo $O_{\mathcal{B}(\mathcal{H})}(t^{-1-\delta'})$:*

$$\exists R(t) = O_{\mathcal{B}(\mathcal{H})}\big(t^{-1-\delta'}\big) \quad s.t. \quad \mathrm{D}_{G(t)} Q_f(t) = \frac{\mathrm{d}}{\mathrm{d}t} Q_f(t) + \mathrm{i}\big[G(t), Q_f(t)\big] \geqslant R(t).$$

iii) *The operators $(W(t) + \alpha(t) + V)Q_f(t)$ and $Q_f(t)(W(t) + \alpha(t) + V)$ are $O_{\mathcal{B}(\mathcal{H})}(t^{-1-\delta'})$.*

Lemma 3.2. *Let $E \in (0, \infty)$. If $e > 0$ is sufficiently small, then there exists a weakly differentiable $Q_p : [1, \infty) \to \mathcal{B}_{sa}(\mathcal{H})$ such that $\|Q_p(t)\|_{\mathcal{B}(\mathcal{H})} \leqslant 1$ and for some $\delta' > 0$*

i)

$$\text{s-}\lim_{t\to\infty} \big(I - Q_p(t)\big)\mathrm{e}^{-\mathrm{i}tH} \chi_{[E-e,E+e]}(H) = 0.$$

ii) *The operators $HQ_p(t)$ and $Q_p(t)H$ are bounded, and*

$$\exists R(t) = O_{\mathcal{B}(\mathcal{H})}\big(t^{-1-\delta'}\big) \quad s.t. \quad \mathrm{D}_H Q_p(t) = \frac{\mathrm{d}}{\mathrm{d}t} Q_p(t) + \mathrm{i}\big[H, Q_p(t)\big] \geqslant R(t).$$

iii) *The operators $(W(t) + \alpha(t) + V)Q_p(t)$ and $Q_p(t)(W(t) + \alpha(t) + V)$ are $O_{\mathcal{B}(\mathcal{H})}(t^{-1-\delta'})$.*

Now we deduce Theorem 1.5 from Lemmas 3.1 and 3.2. The existence and the completeness parts are completely the same and we discuss only the existence part. From Lemma 3.1 ii) and iii) the following statement follows, which combined with Lemma 3.1 i) and a density argument implies the existence of the wave operator.

Lemma 3.3. *Let μ, M, Q_f, δ' be as in Lemma 3.1, and $u \in \chi_{[\mu,M]}(r^2)\mathcal{H}_{aux} \cap C^\infty(M)$. Then for any $\varepsilon > 0$ there exists $t_0 > 0$ such that for any $t, t' \geqslant t_0$ and $v \in C_c^\infty(M)$*

$$\big|\big\langle v, \mathrm{e}^{\mathrm{i}tH} Q_f(t)U(t)u\big\rangle - \big\langle v, \mathrm{e}^{\mathrm{i}t'H} Q_f\big(t'\big)U\big(t'\big)u\big\rangle\big| \leqslant \varepsilon\|v\|.$$

In particular, $\mathrm{e}^{\mathrm{i}tH} Q_f(t)U(t)u$ is a Cauchy sequence as $t \to \infty$.

Proof. Let $\varepsilon > 0$. For any $t \geqslant t' \geqslant 1$ and $v \in C_c^\infty(M)$ we compute, using Lemma 3.1 ii) and iii) and the Schwarz inequality,

$$\begin{aligned}
&\big|\big\langle v, \mathrm{e}^{\mathrm{i}tH} Q_f(t)U(t)u\big\rangle - \big\langle v, \mathrm{e}^{\mathrm{i}t'H} Q_f\big(t'\big)U\big(t'\big)u\big\rangle\big| \\
&\quad = \left| \int_{t'}^{t} \big\{\big\langle v, \mathrm{e}^{\mathrm{i}sH}\mathrm{D}_{G(s)} Q_f(s)U(s)u\big\rangle + \mathrm{i}\big\langle v, \mathrm{e}^{\mathrm{i}sH}\big(W(s) + \alpha(s) + V\big)Q_f(s)U(s)u\big\rangle\big\}\,\mathrm{d}s \right| \\
&\quad \leqslant \left(\int_{t'}^{t} \big\langle v, \mathrm{e}^{\mathrm{i}sH}\big(\mathrm{D}_{G(s)} Q_f(s) - R(s)\big)\mathrm{e}^{-\mathrm{i}sH} v\big\rangle\,\mathrm{d}s \right)^{1/2}
\end{aligned}$$

$$\times\left(\int_{t'}^{t}\langle u,U(s)^*\bigl(\mathrm{D}_{G(s)}Q_{\mathrm{f}}(s)-R(s)\bigr)U(s)u\rangle\,\mathrm{d}s\right)^{1/2}+C\|v\|\|u\|\int_{t'}^{t}s^{-1-\delta'}\,\mathrm{d}s.$$

By Lemma 3.1 iii)

$$\langle v,\mathrm{e}^{\mathrm{i}sH}\bigl(\mathrm{D}_{G(s)}Q_{\mathrm{f}}(s)-R(s)\bigr)\mathrm{e}^{-\mathrm{i}sH}v\rangle=\frac{\mathrm{d}}{\mathrm{d}s}\langle v,\mathrm{e}^{\mathrm{i}sH}Q_{\mathrm{f}}(s)\mathrm{e}^{-\mathrm{i}sH}v\rangle+O\bigl(s^{-1-\delta'}\bigr)\|v\|^2,$$

so that

$$\left(\int_{t'}^{t}\langle v,\mathrm{e}^{\mathrm{i}sH}\bigl(\mathrm{D}_{G(s)}Q_{\mathrm{f}}(s)-R(s)\bigr)\mathrm{e}^{-\mathrm{i}sH}v\rangle\,\mathrm{d}s\right)^{1/2}\leqslant C\|v\|.$$

Similarly, we have

$$\left(\int_{t'}^{t}\langle u,U(s)^*\bigl(\mathrm{D}_{G(s)}Q_{\mathrm{f}}(s)-R(s)\bigr)U(s)u\rangle\,\mathrm{d}s\right)^{1/2}\leqslant C\|u\|,$$

which in particular implies that $\langle u,U(s)^*(\mathrm{D}_{G(s)}Q_{\mathrm{f}}(s)-R(s))U(s)u\rangle\geqslant 0$ is integrable. Hence we obtain

$$\begin{aligned}&\bigl|\langle v,\mathrm{e}^{\mathrm{i}tH}Q_{\mathrm{f}}(t)U(t)u\rangle-\langle v,\mathrm{e}^{\mathrm{i}t'H}Q_{\mathrm{f}}\bigl(t'\bigr)U\bigl(t'\bigr)u\rangle\bigr|\\&\quad\leqslant C\|v\|\left(\int_{t'}^{t}\langle u,U(s)^*\bigl(\mathrm{D}_{G(s)}Q_{\mathrm{f}}(s)-R(s)\bigr)U(s)u\rangle\,\mathrm{d}s\right)^{1/2}+C\|v\|\|u\|\int_{t'}^{t}s^{-1-\delta'}\,\mathrm{d}s.\end{aligned}$$

Since the integrands in the right hand side both are integrable, if we let $t_0>0$ be large enough, we have for $t,t'\geqslant t_0$

$$\bigl|\langle v,\mathrm{e}^{\mathrm{i}tH}Q_{\mathrm{f}}(t)U(t)u\rangle-\langle v,\mathrm{e}^{\mathrm{i}t'H}Q_{\mathrm{f}}\bigl(t'\bigr)U\bigl(t'\bigr)u\rangle\bigr|\leqslant\varepsilon\|v\|.$$

Thus the lemma follows. □

For the existence of the limit $\tilde{\Omega}_+$ the following lemma is sufficient. We omit the proof of the lemma.

Lemma 3.4. *Let $E,e,Q_{\mathrm{p}},\delta'$ be as in Lemma 3.2 and $u\in\chi_{[E-e,E+e]}(H)C_{\mathrm{c}}^\infty(M)$. Then for any $\varepsilon>0$ there exists $t_0>0$ such that for any $t,t'\geqslant t_0$ and $v\in C_{\mathrm{c}}^\infty(M)$*

$$\bigl|\langle v,U(t)^*Q_{\mathrm{p}}(t)\mathrm{e}^{-\mathrm{i}tH}u\rangle-\langle v,U\bigl(t'\bigr)^*Q_{\mathrm{p}}\bigl(t'\bigr)\mathrm{e}^{-\mathrm{i}t'H}u\rangle\bigr|\leqslant\varepsilon\|v\|.$$

In particular, $U(t)^*Q_{\mathrm{p}}(t)\mathrm{e}^{-\mathrm{i}tH}u$ is a Cauchy sequence as $t\to\infty$.

Proof of (1.15), (1.16) and Corollary 1.6. It suffices to show the identity

$$H\Omega_+ = \Omega_+ M_f; \qquad f(x) := 2^{-1} r(x)^2. \tag{3.3}$$

Note that the operator M_f has purely continuous spectrum, given by $[0,\infty)$, so indeed it is a consequence of (3.3) that $\operatorname{Ran}\Omega_+ \subseteq \mathcal{H}_c(H)$. Note that we also have $\operatorname{Ran}\tilde{\Omega}_+ \subseteq \mathcal{H}_{\mathrm{aux}}$. In fact, cf. the RAGE theorem [25], for any $u \in \mathcal{H}_c(H)$

$$\lim_{t\to+\infty} \frac{1}{T}\int_1^T \left\| (P_{\mathrm{aux}})^\perp e^{-itH} u \right\|^2 dt = 0,$$

so that in particular for some sequence t_n

$$t_n \to \infty \quad \text{and} \quad (P_{\mathrm{aux}})^\perp e^{-it_n H} u \to 0$$

as $n \to \infty$. Then, since $U(t)$ is unitary on $(\mathcal{H}_{\mathrm{aux}})^\perp$ and $\mathrm{s}-\lim_{t\to+\infty} U(t)^* e^{-itH} P_c$ exists, we can conclude

$$\mathrm{s}-\lim_{t\to\infty} (P_{\mathrm{aux}})^\perp U(t)^* e^{-itH} P_c = 0.$$

This implies the claim. Therefore (1.15) follows. Note also that given (3.3) the statements (1.16) and Corollary 1.6 are immediate consequences of Theorem 1.5.

For (3.3) we compute for all $s \in \mathbb{R}$

$$\begin{aligned}
\Omega_+ u &= \lim_{t\to\infty} e^{i(t+s)H} e^{iK(t+s,\cdot)} e^{-i\frac{\ln(t+s)}{2}A} P_{\mathrm{aux}} u \\
&= e^{isH} \lim_{t\to\infty} e^{itH} e^{iK(t,\cdot)} e^{i\frac{r^2}{2t^2}(\frac{t^2}{t+s}-t)} e^{-i\frac{\ln t}{2}A} P_{\mathrm{aux}} u \\
&= e^{isH} \lim_{t\to\infty} e^{itH} e^{iK(t,\cdot)} e^{-i\frac{\ln t}{2}A} e^{if(\cdot)(\frac{t^2}{t+s}-t)} P_{\mathrm{aux}} u \\
&= e^{isH} \lim_{t\to\infty} e^{itH} U(t) P_{\mathrm{aux}} e^{-isf(\cdot)} u \\
&= e^{isH} \Omega_+ e^{-isf(\cdot)} u.
\end{aligned}$$

Whence, cf. Stone's theorem [25], $H\Omega_+ \supseteq \Omega_+ M_f$, and therefore also (3.3) holds. □

We end this subsection by also proving Corollary 1.7.

Proof of Corollary 1.7. We note $\operatorname{Ran}\Omega_+ \subseteq \mathcal{H}_c(H)$. Then we compute for all $\phi \in C_c(M)$ and $v \in \mathcal{H}_c(H)$

$$\lim_{t\to\infty} e^{itH} \phi\big(\omega(t,\cdot)\big) e^{-itH} v = \lim_{t\to\infty} e^{itH} U(t)\phi(M_x)U(t)^* e^{-itH} v = \Omega_+ \phi(M_x)\Omega_+^* v,$$

showing the existence of $\phi(\omega_\infty^+) = \mathrm{s} - \lim_{t\to\infty} e^{itH}\phi(\omega(t,\cdot))e^{-itH} P_c$ and the first identity of (1.17).

The existence of the operator $R := r(\omega_\infty^+)$ follows from the fact that the mapping $C_c(\mathbb{R}) \ni \psi \to \phi(\omega_\infty^+) \in \mathcal{B}(\mathcal{H}_c(H))$, $\phi := \psi \circ r$, is a non-degenerate $*$-representation and spectral theory [25]. Clearly $R \geqslant 0$.

We take (using here notation from the next subsection) $\psi_N(s) = \frac{s^2}{2}\chi_{-,0,N}(s)$, $N \in \mathbb{N}$, and take the N-limit in the identity $\psi_N(R)\Omega_+ = \Omega_+ M_{\psi_N \circ r}$. This leads to $\frac{R^2}{2}\Omega_+ \supseteq \Omega_+ M_{r^2/2}$, and whence in combination with (1.16), the second identity of (1.17). In particular the kernel of R is zero. □

3.2. Localization operators in explicit form

The rest of the paper concerns the proofs of Lemmas 3.1 and 3.2. Since the proofs are fairly long, here we first give the explicit forms of Q_{f} and Q_{p}. We also collect here some other (related) constructions.

We denote by $\chi_{a,b,c,d} \in C^\infty(\mathbb{R})$, $-\infty < a < b < c < d < \infty$, a smooth cutoff function such that

$$0 \leqslant \chi_{a,b,c,d} \leqslant 1, \quad \chi_{a,b,c,d} = 1 \quad \text{in a nbh. of } [b,c],$$
$$\chi_{a,b,c,d} = 0 \quad \text{in a nbh. of } \mathbb{R} \setminus (a,d),$$

and that

$$\chi'_{a,b,c,d} \geqslant 0 \quad \text{on } [a,b], \qquad \chi'_{a,b,c,d} \leqslant 0 \quad \text{on } [c,d], \qquad \chi^{1/2}_{a,b,c,d}, \left|\chi'_{a,b,c,d}\right|^{1/2} \in C^\infty(\mathbb{R}).$$

We also assume that the family of these cutoff functions satisfies

$$\chi_{a,b,c,d} + \chi_{c,d,e,f} = \chi_{a,b,e,f},$$
$$\left\|\chi^{(n)}_{a,b,c,d}\right\|_{L^\infty(\mathbb{R})} \leqslant \left\|\chi^{(n)}_{0,1,2,3}\right\|_{L^\infty(\mathbb{R})} \left(\min\{b-a, d-c\}\right)^{-n}.$$

We let $\chi_{-,-,c,d}$ and $\chi_{a,b,+,+}$ be functions with similar properties as above formally given by taking $a = b = -\infty$ and $c = d = +\infty$, respectively. We abbreviate $\chi_{-,c,d} = \chi_{-,-,c,d}$ and $\chi_{a,b,+} = \chi_{a,b,+,+}$. Note that all the above functions may be constructed from $\chi_{0,1,+}$ and $\chi_{-,0,1}$ by a simple translation and scaling procedure as well as multiplication.

Then the localization operators Q_{f} and Q_{p} are realized as the products

$$Q_{\mathrm{f}}(t) = \left(Q_2(t)Q_1(t)\right)^* Q_2(t)Q_1(t), \tag{3.4}$$
$$Q_{\mathrm{p}}(t) = \left(Q_6(t)Q_5(t)Q_4(t)\right)^* Q_6(t)Q_5(t)Q_4(t), \tag{3.5}$$

where we use quantities from the list

$$Q_1(t) = \chi_{\mu_1,\mu,M,M_1}\left(r^2/t^2\right),$$
$$Q_2(t) = \left(I + t^{1+\delta_1}W(t)\right)^{-1/2},$$
$$Q_3 = \chi_{E-2e,E-e,E+e,E+2e}(H),$$
$$Q_4(t) = \chi_{-,2E_1,2E_2}\left(r^2/t^2\right),$$

$$\begin{aligned} Q_5(t) &= \chi_{(1+\delta_3)^2E/2,(1+\delta_2)^2E/2,+}\big(r^2/t^2\big), \\ Q_6(t) &= Q_2(t) = \big(I + t^{1+\delta_1}W(t)\big)^{-1/2}. \end{aligned}$$

The parameters appearing above are chosen as follows: For given $0 < \mu < M < \infty$, if we let μ_1, M_1, δ_1 be any constants such that

$$0 < \mu_1 < \mu < M < M_1 < \infty, \qquad 0 < \delta_1 < \min(\delta, 2\kappa),$$

then Q_{f} satisfies Lemma 3.1. For given $E \in (0, \infty)$ let E_*, δ_* be any constants such that

$$E < E_1 < E_2, \qquad 0 < \delta_3 < \delta_2 < \delta_1 < \min(\delta, 2\kappa),$$

and $e > 0$ small enough accordingly, then Q_{p} satisfies Lemma 3.2.

We shall consider the following modification of r^2 and corresponding quantities. Pick a real-valued $f \in C^\infty(\mathbb{R}_+)$ with $f(s) = 1$ for $s < 1/2$, $f(s) = s$ for $s > 2$ and $f'' \geqslant 0$. Define for any $\epsilon \in (0, 1)$ and all $t \geqslant 1$

$$\begin{aligned} \tilde r^2 &= t^{2-2\epsilon} f\big(t^{2\epsilon-2}r^2\big), \\ \tilde K &= \frac{\tilde r^2}{2t}, \\ \tilde A &= \mathrm{i}\big[H_0, \tilde r^2\big] = \frac{1}{2}\big\{\big(f'(\cdot)\partial_i r^2\big)g^{ij}p_j + p_i^* g^{ij}\big(f'(\cdot)\partial_j r^2\big)\big\}, \\ \tilde G &= \frac{1}{2}p_i^* g^{ij}p_j - \frac{1}{2}(p_i - \partial_i \tilde K)^* g^{ij}(p_j - \partial_j \tilde K). \end{aligned}$$

The latter constructions will be used in Subsection 4.4 to prove the following localization for $e > 0$ chosen sufficiently small

$$\operatorname*{s-\lim}_{t\to\infty}\big(I - Q_3Q_4Q_5^2Q_4Q_3\big)\mathrm{e}^{-\mathrm{i}tH}\chi_{[E-e,E+e]}(H) = 0. \tag{3.6a}$$

For all $u \in \chi_{[E-e,E+e]}(H)\mathcal{H}$:

$$-\int_1^\infty \big\langle \mathrm{e}^{-\mathrm{i}tH}u, \big(\chi^2_{-,2E_1,2E_2}\big)'\big(r^2/t^2\big)\mathrm{e}^{-\mathrm{i}tH}u\big\rangle t^{-1}\,\mathrm{d}t < \infty. \tag{3.6b}$$

For all $u \in \chi_{[E-e,E+e]}(H)\mathcal{H}$:

$$\int_1^\infty \big\langle \mathrm{e}^{-\mathrm{i}tH}u, \big(\chi^2_{(1+\delta_3)^2E/2,(1+\delta_2)^2E/2,+}\big)'\big(r^2/t^2\big)\mathrm{e}^{-\mathrm{i}tH}u\big\rangle t^{-1}\,\mathrm{d}t < \infty. \tag{3.6c}$$

As the reader will see, given (3.6a)–(3.6c), the proofs of Lemmas 3.1 and 3.2 are very similar.

Let T be a self-adjoint operator on a complex Hilbert space $\mathcal{H}$ and $\chi \in C_c^\infty(\mathbb{R})$. We can choose an almost analytic extension $\tilde\chi \in C_c^\infty(\mathbb{C})$, i.e.

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

Then the Helffer–Sjöstrand representation formula reads

$$\chi(T) = \int_{\mathbb{C}} (T - z)^{-1} \, \mathrm{d}\mu(z); \quad \mathrm{d}\mu(z) = -\frac{1}{2\pi \mathrm{i}} \bar{\partial}\tilde{\chi}(z) \, \mathrm{d}z \, \mathrm{d}\bar{z}. \tag{3.7}$$

If S is another operator on $\mathcal{H}$ we are thus lead to the formula

$$\left[S, \chi(T)\right] = \int_{\mathbb{C}} (T - z)^{-1} [T, S] (T - z)^{-1} \, \mathrm{d}\mu(z). \tag{3.8}$$

Another well-known representation formula for T strictly positive reads:

$$T^{-1/2} = \pi^{-1} \int_0^\infty s^{-1/2} (T + s)^{-1} \, \mathrm{d}s. \tag{3.9}$$

4. Verification of properties of localization operators

4.1. Commutator computations

We compute several commutators needed later. We recall that two tensors are denoted by the same symbol if they are related by the identification $TM \cong T^*M$ through the metric tensor, and distinguish them by superscripts and subscripts, for example,

$$\left((\nabla^2 r^2)^{ij}\right) = \left(g^{ik} g^{jl} \left(\nabla^2 r^2\right)_{kl}\right) \in \Gamma(TM \otimes TM).$$

We recall from [8, Lemma 2.5] (this formula can be proved by a straightforward, although somewhat tedious, computation using the compatibility condition (2.21)).

Lemma 4.1. *Let $\phi \in C^\infty(M)$ be given, and define*

$$A_\phi = \mathrm{i}[H_0, \phi] = \frac{1}{2}\left\{(\partial_i \phi) g^{ij} p_j + p_i^* g^{ij} (\partial_j \phi)\right\}.$$

Then, as an operator on $C_\mathrm{c}^\infty(M)$,

$$\mathrm{i}[H_0, A_\phi] = p_i^* \left(\nabla^2 \phi\right)^{ij} p_j - \frac{1}{4} \Delta^2 \phi.$$

Let A be the self-adjoint operator defined by (1.8c), i.e. we take $\phi = r^2$ above. From Lemma 4.1 we thus obtain

Corollary 4.2. *As a quadratic form on $C_c^\infty(M)$,*

$$\mathrm{i}[H, A] = p_i^*\big(\nabla^2 r^2\big)^{ij} p_j + \gamma_i g^{ij}\partial_j + \partial_i^* g^{ij}\gamma_j + \gamma_0; \tag{4.1a}$$

$$\gamma_i = \big(\partial_i r^2\big)V + \frac{1}{4}\big(\partial_i \Delta r^2\big), \tag{4.1b}$$

$$\gamma_0 = \big(\Delta r^2\big)V. \tag{4.1c}$$

In particular, for any $\varepsilon > 0$ there exists $\gamma_\varepsilon = \gamma_\varepsilon(x) = O(r^{-\min\{2\eta, 1+2\kappa\}})$ such that

$$\begin{aligned}\mathrm{i}[H, A] &\geqslant p_i^*\big\{\big(\nabla^2 r^2\big)^{ij} - \varepsilon g^{ij}\big\} p_j + \gamma_\varepsilon \\ &\geqslant 2(1+\delta-\varepsilon)H_0 - C H_{r_1} + \gamma_\varepsilon,\end{aligned} \tag{4.2}$$

where $H_{r_1} = \frac{1}{2} p_i^* \chi_{-,r_0,r_1}(r) g^{ij} p_j$, $r_1 > r_0$.

Proof. Eqs. (4.1a)–(4.1c) follow from Lemma 4.1 and

$$\mathrm{i}[V, A] = V\big(\partial_j r^2\big) g^{ij}\partial_i + \partial_i^* g^{ij}\big(\partial_j r^2\big)V + \big(\Delta r^2\big)V.$$

If we use (1.13) and

$$\gamma_i g^{ij}\partial_j + \partial_i^* g^{ij}\gamma_j + \gamma_0 \geqslant -\varepsilon\partial_i^* g^{ij}\partial_j + \gamma_\varepsilon; \quad \gamma_\varepsilon := -\varepsilon^{-1} g^{ij}\gamma_i\gamma_j + \gamma_0,$$

then the latter assertion of the corollary follows. Note that indeed since $|\partial_r \Delta r^2| \leqslant C\langle r\rangle^{-1/2-\kappa}$ we obtain by integrating in r that $\Delta r^2 = O(r^{1/2-\kappa})$. □

Corollary 4.3. *As a quadratic form on $C_c^\infty(M)$,*

$$\begin{aligned}\mathrm{D}_{H_0} W &= -\frac{1}{2t}(p_i - \partial_i K)^*\big(\nabla^2 r^2\big)^{ij}(p_j - \partial_j K) + \tilde\gamma_i^* g^{ij}(p_j - \partial_j K) + (p_i - \partial_i K)^* g^{ij}\tilde\gamma_j; \\ \tilde\gamma_i &= \frac{\mathrm{i}}{8t}\big(\partial_i \Delta r^2\big) - \frac{1}{2}(\partial_i \alpha).\end{aligned}$$

Proof. We have

$$\mathrm{D}_{H_0} W = \frac{\mathrm{d}}{\mathrm{d}t} W + \mathrm{i}[H_0, W]. \tag{4.3}$$

For the first term substitute

$$W = H_0 - \frac{1}{2}(\partial_i K) g^{ij} p_j - \frac{1}{2} p_i^* g^{ij}(\partial_j K) + \frac{1}{2} g^{ij}(\partial_i K)(\partial_j K),$$

and then we obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}W = \frac{1}{4}\big(\partial_i g^{kl}(\partial_k K)(\partial_l K)\big)g^{ij}p_j + \frac{1}{4}p_i^* g^{ij}\big(\partial_j g^{kl}(\partial_k K)(\partial_l K)\big)$$
$$- \frac{1}{2}g^{ij}(\partial_i K)\big(\partial_j g^{kl}(\partial_k K)(\partial_l K)\big) - \frac{1}{2}(\partial_i\alpha)g^{ij}p_j$$
$$- \frac{1}{2}p_i^* g^{ij}(\partial_j\alpha) + g^{ij}(\partial_i K)(\partial_j\alpha). \tag{4.4}$$

For the second term of (4.3) we substitute

$$W = H_0 - \frac{1}{2t}A + \frac{1}{2}g^{ij}(\partial_i K)(\partial_j K),$$

and then by Lemma 4.1

$$\mathrm{i}[H_0, W] = -\frac{1}{2t}p_i^*\big(\nabla^2 r^2\big)^{ij}p_j - \frac{\mathrm{i}}{8t}\big(\partial_i\Delta r^2\big)g^{ij}p_j + \frac{\mathrm{i}}{8t}p_i^* g^{ij}\big(\partial_j\Delta r^2\big)$$
$$+ \frac{1}{4}\big(\partial_i g^{kl}(\partial_k K)(\partial_l K)\big)g^{ij}p_j + \frac{1}{4}p_i^* g^{ij}\big(\partial_j g^{kl}(\partial_k K)(\partial_l K)\big). \tag{4.5}$$

Noting the equation, cf. (2.22),

$$\big(\partial_j g^{kl}(\partial_k K)(\partial_l K)\big) = 2g^{kl}(\nabla K)^2_{jk}(\partial_l K), \tag{4.6}$$

we obtain the assertion from (4.3)–(4.5). □

Introduce the "radial momentum" (the name of this operator is justified by its action on functions supported in E)

$$p_r = (\partial_k r)g^{kl}p_l. \tag{4.7}$$

Lemma 4.4. *For any real-valued $\chi \in C^\infty(\mathbb{R})$ with $\chi' \in C_c^\infty(\mathbb{R}_+)$ define $p_\chi = \chi(r)p_r$. Then as quadratic forms on $\mathcal{D}(H_0^{1/2})$*

$$p_\chi^* = p_\chi - \mathrm{i}\big(\chi(r)\Delta r + \chi'(r)\big), \tag{4.8a}$$
$$p_\chi p_\chi^* = p_\chi^* p_\chi + \tilde\chi; \quad \tilde\chi = \tilde\chi(x) := -\chi\big(\partial_r\big(\chi(r)\Delta r + \chi'(r)\big)\big), \tag{4.8b}$$
$$p_\chi^* p_\chi \leqslant 2\sup\chi^2 H_0, \tag{4.8c}$$
$$p_\chi p_\chi^* \leqslant 2\sup\chi^2 H_0 + \sup\tilde\chi. \tag{4.8d}$$

Proof. Compute $p_\chi^* = p_\chi + \mathrm{i}(\partial_i^* g^{ij}(\partial_j r)\chi(r)) = p_\chi - \mathrm{i}(\chi(r)\Delta r + \chi'(r))$ yielding (4.8a). We obtain (4.8b) from (4.8a) by inserting and commuting through. The estimate (4.8c) follows from the Cauchy Schwarz inequality and the fact that $|\nabla r| \leqslant 1$. The estimate (4.8d) follows from (4.8b) and (4.8c). □

In the proof of Lemma 4.15 we need the following technical result which involves the construction $\tilde G$ of Subsection 3.2 given in terms of any $\epsilon \in (0, 1)$.

Lemma 4.5. *There exists $\epsilon' = \epsilon'(\epsilon, \kappa, \eta) > 0$ such that as a quadratic form on $C_c^\infty(M)$*

$$\mathrm{D}_H \tilde{G} \geqslant \frac{1}{2t}(p_i - \partial_i K)^* f'(\cdot)\big(\nabla^2 r^2\big)^{ij}(p_j - \partial_j K) - Ct^{-\epsilon'-1}H + O\big(t^{-\epsilon'-1}\big).$$

Proof. We proceed by computing, mimicking the proof of Corollaries 4.2 and 4.3,

$$\mathrm{D}_H \tilde{G} = \frac{\mathrm{d}}{\mathrm{d}t}\tilde{G} + \frac{\mathrm{i}}{2t}[H, \tilde{A}] - \frac{\mathrm{i}}{2}\big[H_0, g^{ij}(\partial_i \tilde{K})(\partial_j \tilde{K})\big].$$

By (4.6) and $(\partial_i \tilde{K}) = f'(\cdot)(\partial_i K)$

$$(\partial_t \partial_i \tilde{K}) = -f'(\cdot)g^{kl}\big(\nabla^2 K\big)_{ik}(\partial_l K) + f'(\cdot)(\partial_i \alpha) + (2\epsilon - 2)t^{2\epsilon-3}r^2 f''(\cdot)(\partial_i K),$$

so that we obtain

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\tilde{G} &= -\frac{1}{2}(\partial_i K)f'(\cdot)\big(\nabla^2 K\big)^{ij}(p_j - \partial_j \tilde{K}) \\ &\quad + \frac{1}{2}\big\{f'(\cdot)(\partial_i \alpha) + (2\epsilon - 2)t^{2\epsilon-3}r^2 f''(\cdot)(\partial_i K)\big\}g^{ij}(p_j - \partial_j \tilde{K}) + \mathrm{h.c.} \\ &= -\frac{1}{2}(\partial_i K)f'(\cdot)\big(\nabla^2 K\big)^{ij}(p_j - \partial_j K) \\ &\quad - \frac{1}{2}f'(\cdot)(\partial_i \alpha)g^{ij}p_j + O\big(t^{-\epsilon-1}\big)p_r + O\big(t^{-2\epsilon-1}\big) + \mathrm{h.c.}\end{aligned}$$

Upon replacing r^2 by $\tilde{K}$ in Corollary 4.2, we have

$$\begin{aligned}\frac{\mathrm{i}}{2t}[H, \tilde{A}] &= p_i^*\big(\nabla^2 \tilde{K}\big)^{ij}p_j - 2\,\mathrm{Im}\left\{\left((\partial_i \tilde{K})V + \frac{1}{4}(\partial_i \Delta \tilde{K})\right)g^{ij}p_j\right\} + (\Delta \tilde{K})V \\ &\geqslant p_i^* f'(\cdot)\big(\nabla^2 K\big)^{ij}p_j + \mathrm{Im}\big\{O\big(t^{\max\{-(1-\epsilon)\eta-1, \epsilon-2, -(1/2+\kappa)(1-\epsilon)-1\}}\big)p_r\big\} \\ &\quad - \frac{1}{2}\mathrm{Im}\big\{f'(\cdot)(\partial_i \Delta K)g^{ij}p_j\big\} + O\big(t^{-(1-\epsilon)(1/2+\kappa+\eta)-1}\big),\end{aligned}$$

where in the last step we used the inequality for matrices:

$$\big(\nabla^2 \tilde{r}^2\big)_{ij} = f'(\cdot)\big(\nabla^2 r^2\big)_{ij} + t^{2\epsilon-2}f''(\cdot)\big(\partial_i r^2\big)\big(\partial_j r^2\big) \geqslant f'(\cdot)\big(\nabla^2 r^2\big)_{ij}.$$

By (4.6) and $(\partial_i \tilde{K}) = f'(\cdot)(\partial_i K)$ again

$$\begin{aligned}-\frac{\mathrm{i}}{2}\big[H_0, g^{ij}(\partial_i \tilde{K})(\partial_j \tilde{K})\big] &= -\frac{1}{4}\big(\partial_i f'(\cdot)^2 g^{kl}(\partial_k K)(\partial_l K)\big)g^{ij}p_j + \mathrm{h.c.} \\ &= -\frac{1}{2}(\partial_i K)f'(\cdot)^2\big(\nabla^2 K\big)^{ij}p_j + O\big(t^{-\epsilon-1}\big)p_r + \mathrm{h.c.} \\ &= -\frac{1}{2}(\partial_i K)f'(\cdot)\big(\nabla^2 K\big)^{ij}p_j + O\big(t^{-\epsilon-1}\big)p_r + \mathrm{h.c.},\end{aligned}$$

where we used that for all large t the function $f'(\cdot)$ is supported in E and whence

$$(\partial_i K)f'(\cdot)^2\big(\nabla^2 K\big)^{ij}p_j = \frac{r}{t^2}f'(\cdot)^2 p_r = (\partial_i K)\big(f'(\cdot)\nabla^2 K\big)^{ij}p_j + O\big(t^{-\epsilon-1}\big)p_r.$$

We sum and obtain the assertion. □

4.2. Further commutator computations

In this subsection we collect some further preliminary commutator bounds.

Lemma 4.6. *Let $\epsilon > 0$ and $0 < c < d < a < b$ be given. Then uniformly in $t, N \geqslant 1$*

$$\big\|B\chi_{-,c,d}(r/t)\big(I + t^{2-2\epsilon}N^{-1}H_0\big)^{-1}\chi_{a,b,+}(r/t)\big\| \leqslant C_n\big(t^{\epsilon}N^{1/2}\big)^{-n}, \tag{4.9}$$

where either $B = B_1 = I$ or $B = B_2 = t^{1-\epsilon}N^{-1/2}p_r$ (with p_r given by (4.7)) and $n \in \mathbb{N}\cup\{0\}$.

Proof. Let $T = I + t^{2-2\epsilon}N^{-1}H_0$. For $n = 0$ we note that

$$\big[B_2, \chi_{-,c,d}(\cdot)\big] = -\mathrm{i}t^{-\varepsilon}N^{-1/2}\chi'_{-,c,d}(\cdot)$$

which obviously is bounded uniformly in $t \geqslant 1$. Moreover

$$\big\|\chi_{-,c,d}(\cdot)B_2T^{-1}\big\| \leqslant \big\|B_2T^{-1}\big\| \leqslant \sqrt{2}\big(\sup|\nabla r|\big)t^{1-\epsilon}N^{-1/2}\big\|H_0^{1/2}T^{-1}\big\| \leqslant 1/\sqrt{2}. \tag{4.10}$$

This proves (4.9) for $n = 0$.

For $n \geqslant 1$ we proceed by induction (using the freedom of using new localization functions) first computing

$$B\chi_{-,c,d}(\cdot)T^{-1}\chi_{a,b,+}(\cdot) = -\frac{\mathrm{i}}{2}t^{1-2\epsilon}N^{-1}BT^{-1}\big(p_r^*\chi'_{-,c,d}(\cdot) + \chi'_{-,c,d}(\cdot)p_r\big)T^{-1}\chi_{a,b,+}(\cdot).$$

Now we can freely introduce a factor $\chi_{-,e,f}(\cdot)$ with $d < e < f < a$ in front of the last factor T^{-1} to the right. By induction we have

$$\big\|B\chi_{-,e,f}(\cdot)T^{-1}\chi_{a,b,+}\big\| \leqslant C\big(t^{\epsilon}N^{1/2}\big)^{-(n-1)} \quad \text{uniformly in } t, N \geqslant 1. \tag{4.11}$$

Whence we are left with bounding

$$\big\|t^{1-2\epsilon}N^{-1}BT^{-1}p_r^*\chi'_{-,c,d}(\cdot)\big\| \leqslant Ct^{-\epsilon}N^{-1/2} \quad \text{uniformly in } t, N \geqslant 1, \tag{4.12a}$$

$$\big\|t^{-\epsilon}N^{-1/2}BT^{-1}\chi'_{-,c,d}(\cdot)\big\| \leqslant Ct^{-\epsilon}N^{-1/2} \quad \text{uniformly in } t, N \geqslant 1. \tag{4.12b}$$

Clearly (4.12a) and (4.12b) in turn follow from the following bound:

$$\big\|B_iT^{-1}B_j^*\big\| \leqslant 2, \quad i, j \in \{1, 2\}. \tag{4.13}$$

But as in (4.10)

$$\|B_1 T^{-1} B_j^*\| = \|T^{-1} B_j^*\| = \|B_j T^{-1}\| \leqslant 1,$$

while

$$\|B_2 T^{-1} B_j^*\| \leqslant \|B_2 T^{-1/2}\| \times \|T^{-1/2} B_j^*\| \leqslant 2.$$

So indeed (4.13) is shown, and the proof of the lemma is complete. □

Corollary 4.7. *For $\epsilon > 0$, $\chi \in C^\infty(\mathbb{R})$ with $\chi' \in C_c^\infty(\mathbb{R}_+)$ and for B given as in Lemma 4.6 we have uniformly in $t, N \geqslant 1$*

$$\|B[\chi(r/t), (I + t^{2-2\epsilon} N^{-1} H_0)^{-1}]\| \leqslant C t^{-\epsilon}. \tag{4.14}$$

Lemma 4.8. *For any real-valued $\chi \in C^\infty(\mathbb{R})$ with $\chi' \in C_c^\infty(\mathbb{R}_+)$ we have uniformly in $t \geqslant 1$*

$$\|\langle H\rangle^{1/2}[Q_3, \chi(r/t)]\langle H\rangle^{1/2}\| \leqslant C \sup|\chi'| t^{-1}, \tag{4.15a}$$

$$\|\langle H\rangle^{1/2}[Q_3, (\chi'(r/t) p_r + h.c.)]\langle H\rangle^{1/2}\| \leqslant C_{\chi'} t^{-1/2-\kappa}. \tag{4.15b}$$

Proof. We calculate

$$\mathrm{i}[H, \chi(r/t)] = \frac{1}{2t}\chi'(r/t) p_r + \text{h.c.} \tag{4.16}$$

Hence in combination with (3.8) and (4.8c)

$$\begin{aligned}
\|\langle H\rangle^{1/2}[Q_3, \chi(r/t)]\langle H\rangle^{1/2}\| &\leqslant C_1 t^{-1} \int_{\mathbb{C}} \|\chi'(r/t) p_r \langle H\rangle^{-1/2}\| \frac{\langle z\rangle^2}{|\operatorname{Im} z|^2} |\mathrm{d}\mu(z)| \\
&\leqslant C_2 \sup|\chi'| t^{-1} \int_{\mathbb{C}} \frac{\langle z\rangle^2}{|\operatorname{Im} z|^2} |\mathrm{d}\mu(z)| = C_3 \sup|\chi'| t^{-1},
\end{aligned}$$

showing (4.15a).

As for (4.15b) we rewrite

$$2 \operatorname{Re} p_{\chi'} = t\{(\partial_i \chi(r/t)) g^{ij} p_j + p_i^* g^{ij} (\partial_j \chi(r/t))\},$$

and apply Corollary 4.2 with the expression r^2 replaced by $2t\chi(r/t)$. Now we note, cf. (1.6b), that

$$t\nabla^2 \chi(\cdot/t) = t^{-1} \chi''(\cdot/t)\, \mathrm{d}r \otimes \mathrm{d}r + \chi'(\cdot/t) \nabla^2 r,$$

$$0 \leqslant \nabla^2 r \leqslant (\Delta r) g \leqslant C_1 \langle r\rangle^{-1/2-\kappa} g, \quad r \geqslant r_0,$$

leading to the estimates

$$-C_2 t^{-1/2-\kappa} g \leqslant 2t\nabla^2 \chi(\cdot/t) \leqslant C_2 t^{-1/2-\kappa} g, \quad t \geqslant 1.$$

Using again (3.8) this leads to (4.15b). □

In the proof of Lemma 4.16 we need the following technical result.

Lemma 4.9. *For all real-valued $\chi, \hat\chi \in C^\infty(\mathbb{R})$ vanishing for large enough argument and with $\chi', \hat\chi' \in C_c^\infty(\mathbb{R}_+)$*

$$\operatorname{Re}\bigl(T^*\bigl(\operatorname{Re} p_{\hat\chi'(r/t)} - r/t\,\hat\chi'(r/t)\bigr)\bigr) = T^*\hat\chi'(r/t)(p_r - r/t) + O\bigl(t^{-1/2-\kappa}\bigr), \tag{4.17}$$

where $T = t^{-1}A\chi(r/t)Q_3$.

Proof. Introducing $\gamma = T^*(\operatorname{Re} p_{\hat\chi'(r/t)} - r/t\,\hat\chi'(r/t))$ and noting that $\|T\|$ is uniformly bounded we obtain from (1.6b) and (4.8a) that γ has the form of the right hand side of (4.17). It remains to show that

$$\gamma^* = \gamma + O\bigl(t^{-1/2-\kappa}\bigr). \tag{4.18}$$

For that we write

$$\gamma^* = (\operatorname{Re} p_{\hat\chi'})\frac{A}{t}\chi Q_3 - \bigl(r/t\,\hat\chi'\bigr)\frac{A}{t}\chi Q_3,$$

and commute the four factors for each of the two terms on the right hand side. Rearranging we then get γ plus contributions from commutators. The latter are treated using repeatedly Corollary 4.2 and (4.16). The most difficult parts arise from commuting the operators $\operatorname{Re} p_{\hat\chi'}$ or $\frac{A}{t}$ through the factors of Q_3. Here we shall only explain how to treat the first term above (the most difficult one). We have

$$(\operatorname{Re} p_{\hat\chi'})\frac{A}{t}\chi Q_3 = (\operatorname{Re} p_{\hat\chi'})Q_3\frac{A}{t}\chi + (\operatorname{Re} p_{\hat\chi'})\left[\frac{A}{t}\chi, Q_3\right], \tag{4.19}$$

we represent (introducing here for convenience a suitable function $\tilde\chi$ with $\tilde\chi\chi = \chi$)

$$(\operatorname{Re} p_{\hat\chi'})\left[\frac{A}{t}\chi, Q_3\right] = \int_{\mathbb{C}} (\operatorname{Re} p_{\hat\chi'})(H-z)^{-1}\left(\tilde\chi\left[H, \frac{A}{t}\right]\chi + \frac{A}{t}[H,\chi]\right)(H-z)^{-1}\,\mathrm{d}\mu(z),$$

and then we use Corollary 4.2 and estimate inside the integral. Note the estimates, cf. Conditions 1.2 and 1.3,

$$0 \leqslant \nabla^2 r^2 \leqslant \bigl(\Delta r^2\bigr)g \leqslant C\langle r\rangle^{1/2-\kappa}g, \quad r \geqslant r_0. \tag{4.20}$$

Since we have the factors $\tilde\chi$ and χ to the left and to the right of $[H, \frac{A}{t}]$, respectively, the Cauchy Schwarz inequality and these bounds lead to the bound $O(t^{-1/2-\kappa})$ of the second term to the right in (4.19).

Similarly for the first term in (4.19) we write

$$(\operatorname{Re} p_{\hat\chi'})Q_3\frac{A}{t}\chi = Q_3(\operatorname{Re} p_{\hat\chi'})\frac{A}{t}\chi + [\operatorname{Re} p_{\hat\chi'}, Q_3]\frac{A}{t}\chi. \tag{4.21}$$

The second term of (4.21) is $O(t^{-1/2-\kappa})$ due to (4.15b).

Finally for the first term in (4.21) we have

$$Q_3(\operatorname{Re} p_{\hat{\chi}'})\frac{A}{t}\chi = Q_3\chi\frac{A}{t}\operatorname{Re} p_{\hat{\chi}'} + Q_3\chi\left[\operatorname{Re} p_{\hat{\chi}'}, \frac{A}{t}\right] + O\big(t^{-1/2-\kappa}\big).$$

Only the middle term needs examination. We show that it is also $O(t^{-1/2-\kappa})$ by introducing $\tilde{\chi}(s) := \hat{\chi}'(s) - s\hat{\chi}''(s)$ and computing the adjoint

$$\begin{aligned}-\left[\operatorname{Re} p_{\hat{\chi}'}, \frac{A}{t}\right]\chi Q_3 &= \left(-\frac{2}{t}[p_{\hat{\chi}'}, rp_r] + O\big(t^{-3/2-\kappa}\big)\right)\chi Q_3\\ &= \left(\frac{2\mathrm{i}}{t}p_{\tilde{\chi}(r/t)} + O\big(t^{-3/2-\kappa}\big)\right)\chi Q_3.\end{aligned}$$

Due to (4.8c) the norm of this expression is in fact bounded by Ct^{-1}. □

4.3. Proof of Lemma 3.1

In this section we let $0 < \mu < M < \infty$, and choose $\mu_1, M_1, \delta_1, Q_1, Q_2$ as in Subsection 3.2. Since $\mathrm{e}^{-\mathrm{i}K(t,\cdot)}U(t)$ is the dilation, the following statement is obvious.

Lemma 4.10. *For all $u \in \chi_{[\mu,M]}(r^2)\mathcal{H}_{\mathrm{aux}}$*

$$(1 - Q_1)Uu = 0.$$

This lemma can be proved also by the (somewhat formal) equation

$$\mathrm{D}_G Q_1 P_{\mathrm{aux}} = 0. \tag{4.22}$$

Eq. (4.22) is obtained by a direct computation.

Lemma 4.11. *For all $u \in \chi_{[\mu,M]}(r^2)\mathcal{H}_{\mathrm{aux}}$*

$$\lim_{t\to\infty}\big\langle Uu, \big(I - Q_2^2\big)Uu\big\rangle = 0. \tag{4.23}$$

Proof. Fix $\bar{\delta} \in (\delta_1, \delta)$ with $\bar{\delta} < 2\kappa$, and fix $u \in \chi_{[\mu,M]}(r^2)\mathcal{H}_{\mathrm{aux}} \cap C^\infty(M)$ (by density (4.23) for any such state suffices). Set for $N \geqslant 1$

$$T_N = T_N(t) = I + t^{1+\bar{\delta}}N^{-1}W(t),$$

and note that

$$\mathrm{e}^{-\mathrm{i}K}T_N\mathrm{e}^{\mathrm{i}K} = I + t^{1+\bar{\delta}}N^{-1}H_0. \tag{4.24}$$

We need to show that with $N(t) := t^{\bar{\delta}-\delta_1}$

$$\lim_{t\to\infty}\big\langle Uu, \big(I - T_{N(t)}^{-1}\big)Uu\big\rangle = 0.$$

It suffices to show that there exists $R(t) \in \mathcal{B}(\mathcal{H})$ such that

$$\int_{t_0}^{\infty} \bigl|\langle U(t)u, R(t)U(t)u\rangle\bigr| \,\mathrm{d}t = o\bigl(t_0^0\bigr) \quad \text{uniformly in } N \geqslant 1, \tag{4.25a}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\bigl\langle U(t)u, \bigl(I - T_N^{-1}(t)\bigr)U(t)u\bigr\rangle \leqslant \bigl\langle U(t)u, R(t)U(t)u\bigr\rangle. \tag{4.25b}$$

In fact from (4.25a) and (4.25b) it follows that for any $\varepsilon > 0$ there exists $t_0 \geqslant 1$ such that for all $t \geqslant t_0$ and $N \geqslant 1$

$$\bigl\langle U(t)u, \bigl(I - T_N^{-1}(t)\bigr)U(t)u\bigr\rangle \leqslant \bigl\langle U(t_0)u, \bigl(I - T_N^{-1}(t_0)\bigr)U(t_0)u\bigr\rangle + \varepsilon.$$

Then for all $N \geqslant 1$ large enough we have for all $t \geqslant t_0$

$$0 \leqslant \bigl\langle U(t)u, \bigl(I - T_N^{-1}\bigr)U(t)u\bigr\rangle \leqslant 2\varepsilon.$$

In particular we can take $N = t^{\bar{\delta}-\delta_1}$, and indeed we obtain that

$$0 \leqslant \bigl\langle U(t)u, \bigl(I - T_{N(t)}^{-1}\bigr)U(t)u\bigr\rangle \leqslant 2\varepsilon \quad \text{for all sufficiently large } t.$$

Hence we only need to prove (4.25a) and (4.25b). We have

$$\frac{\mathrm{d}}{\mathrm{d}t} U^*\bigl(1 - T_N^{-1}\bigr)U = U^*\bigl(-\mathrm{D}_G T_N^{-1}\bigr)U = U^* T_N^{-1}\bigl(\mathrm{D}_{H_0} T_N - \mathrm{i}[\alpha, T_N]\bigr)T_N^{-1}U. \tag{4.26}$$

By Corollary 4.3 (in combination with an approximation argument), (1.3) and the Cauchy Schwarz inequality it follows for $r_1 > r_0$

$$\mathrm{D}_{H_0} T_N \leqslant C t^{\bar{\delta}} N^{-1} (p_i - \partial_i K)^* \chi_{-,r_0,r_1}(r) g^{ij} (p_j - \partial_j K) + \frac{2}{\delta - \bar{\delta}} t^{2+\bar{\delta}} N^{-1} |\tilde{\gamma}|^2.$$

Since $\operatorname{supp} \chi_{-,r_0,r_1} \subset (-\infty, r_1]$, we obtain by using (4.24) and Lemma 4.6

$$\begin{aligned} &t^{\bar{\delta}} N^{-1} \bigl\| Q_1^* T_N^{-1} (p_i - \partial_i K)^* \chi_{-,r_0,r_1}(r) g^{ij} (p_j - \partial_j K) T_N^{-1} Q_1 \bigr\| \\ &\quad \leqslant C t^{-2} \quad \text{uniformly in } N \geqslant 1. \end{aligned} \tag{4.27}$$

We claim

$$t^{2+\bar{\delta}} N^{-1} \bigl\| Q_1^* T_N^{-1} |\tilde{\gamma}|^2 T_N^{-1} Q_1 \bigr\| \leqslant C t^{-1+\bar{\delta}-2\kappa} \quad \text{uniformly in } N \geqslant 1. \tag{4.28}$$

Choose $0 < \mu_3 < \mu_2 < \mu_1$ (with μ_1 as given). Due to (1.6a) obviously

$$t^{2+\bar{\delta}} N^{-1} \bigl\| \chi_{\mu_3,\mu_2,+}\bigl(r^2/t^2\bigr) |\tilde{\gamma}|^2 \bigr\| \leqslant C t^{-1+\bar{\delta}-2\kappa} \quad \text{uniformly in } N \geqslant 1, \tag{4.29a}$$

which is agreeable with (4.28). On the other hand due to (1.6a), (4.24) and Lemma 4.6 (used with $2\epsilon = 1 - \bar{\delta}$ there) we can estimate

$$t^{2+\bar{\delta}} N^{-1} \big\| Q_1^* T_N^{-1} \chi_{-,\mu_3,\mu_2}\big(r^2/t^2\big)|\tilde{\gamma}|^2 T_N^{-1} Q_1 \big\| \leqslant C t^{-2} \quad \text{uniformly in } N \geqslant 1, \tag{4.29b}$$

which also agrees with (4.28). Using the bound $|\mathrm{d}\alpha| \leqslant C t^{-2}$, cf. (3.2), we obtain for the second term in (4.26)

$$\big\| T_N^{-1} \mathrm{i}[\alpha, T_N]) T_N^{-1} \big\| \leqslant C t^{-3/2+\bar{\delta}/2} \quad \text{uniformly in } N \geqslant 1. \tag{4.30}$$

The combination of the bounds (4.29a) and (4.29b) implies (4.28) and therefore, together with (4.27) and (4.30), also (4.25a) and (4.25b). □

Proof of Lemma 3.1. Consider the operator Q_{f} given by (3.4). The property i) of Lemma 3.1 for this operator follows from Lemmas 4.10 and 4.11. By mimicking the proof of Lemma 4.11 we obtain the property ii) for any $\delta' \leqslant 2\kappa - \delta_1$. Finally the property $(W(t) + V + \alpha(t))Q_{\mathrm{f}}(t) \in O_{\mathcal{B}(\mathcal{H})}(t^{-1-\delta'})$ of iii), here possibly $\delta' > 0$ taken smaller, is proved by first computing

$$\begin{aligned}(W + V + \alpha)Q_{\mathrm{f}} = t^{-1-\delta_1} Q_1\big(t^{1+\delta_1} W Q_2\big) Q_2 Q_1 \\ + [W, Q_1] Q_2^2 Q_1 + t^{-1-\eta}\big(t^{1+\eta} V Q_1\big) Q_2^2 Q_1 + \alpha Q_{\mathrm{f}}.\end{aligned}$$

The first, third and fourth terms agree with iii). As for the second term we compute

$$[W, Q_1] = -\mathrm{i}\chi'_{\mu_1,\mu,M,M_1}\big(r^2/t^2\big)\frac{r}{t^2}(\partial_i r) g^{ij}(p_j - \partial_j K) - \text{h.c.}$$

Whence we can write

$$[W, Q_1] Q_2 = \mathrm{e}^{\mathrm{i}K}\big(\big(-\mathrm{i}t^{-1}\chi(r/t) p_r - \text{h.c.}\big)\big(I + t^{1+\delta_1} H_0\big)^{-1/2}\big)\mathrm{e}^{-\mathrm{i}K}$$

with $\chi(s) = s\chi'_{\mu_1,\mu,M,M_1}(s^2)$. By using this identity, Lemma 4.4 and (1.6b) we obtain

$$\big\|[W, Q_1] Q_2\big\|^2 \leqslant C\big(t^{-3-\delta_1} + t^{-3-2\kappa}\big). \qquad \square$$

4.4. *Preliminary localization for perturbed dynamics*

In this subsection we first study various preliminary localization properties of the perturbed dynamics. We prove maximal and minimal velocity bounds and in particular the properties (3.6a)–(3.6c). Similar properties were also used in the proof of Lemma 3.1, cf. Lemma 4.10. However the proofs for the perturbed dynamics are somewhat technical. Since all we need from this subsection for the proof of Lemma 3.2 is in fact the properties (3.6a)–(3.6c) the reader might prefer to read the next subsection (presenting a proof of Lemma 3.2 along the lines of the proof of Lemma 3.1) before coming back to the present one. The subsection depends on [12,26] although the presentation is self-contained.

Let $E \in (0, \infty)$ and we fix Q_* and the parameters E_*, δ_* as in Subsection 3.2. The small parameter $e > 0$ will be determined in this section. Possibly we will retake it smaller each time it appears. The following type of result is called a *Mourre estimate* in the literature since the appearance of such estimate in the seminal work [24]. The reader should keep in mind though that the commutator in Corollary 4.2 does not conform with the conditions of [24] since under our conditions it might not be bounded relative to H (not even in the form sense). At this point we remark that Donnelly [8] indeed uses Mourre theory under his geometric conditions. In fact our conditions do not conform neither with more recent refinement of Mourre theory as a method to provide the limiting absorption principle [23,11,9]. However as the reader will see we are not going to use this theory, or more generally limiting absorption bounds, only the following reminiscence.

Lemma 4.12. *For $e > 0$ sufficiently small, as a form estimate on $C_c^\infty(M)$,*

$$\mathrm{i}[H, A] \geqslant 2(1+\delta_1)E - C(I - Q_3)(H_{r_1} + 1)(I - Q_3). \tag{4.31}$$

Proof. Fix $\varepsilon > 0$ such that $\delta_1 < \delta - 3\varepsilon$. By (1.3) and (4.2)

$$\begin{aligned}\mathrm{i}[H, A] &\geqslant 2(1+\delta-\varepsilon)H_0 - CH_{r_1} + \gamma_\varepsilon = 2(1+\delta-\varepsilon)H - CH_{r_1} + o\big(\langle r\rangle^0\big)\\ &\geqslant 2(1+\delta-2\varepsilon)Q_3HQ_3 - C_1(\varepsilon)(I-Q_3)(H_{r_1}+1)(I-Q_3) + K;\\ K &= Q_3\big\{-CH_{r_1} + o\big(\langle r\rangle^0\big)\big\}Q_3.\end{aligned}$$

Since K is compact and $E \notin \sigma_{\mathrm{pp}}(H)$, we can make $\|K\|_{\mathcal{B}(\mathcal{H})}$ arbitrary small by letting $e > 0$ small. Hence if $e > 0$ is sufficiently small we obtain

$$\begin{aligned}\mathrm{i}[H, A] &\geqslant 2(1+\delta-3\varepsilon)(E-2e) - C_2(\varepsilon)(I-Q_3)(H_{r_1}+1)(I-Q_3)\\ &\geqslant 2(1+\delta_1)E - C_2(\varepsilon)(I-Q_3)(H_{r_1}+1)(I-Q_3). \qquad \Box\end{aligned}$$

The following type of result is called a *maximal velocity bound* in the literature. We shall present a somewhat different proof than seen in for example [3,12]. It is more in the spirit of the proof of Lemma 4.11.

Lemma 4.13. *If $e > 0$ is sufficiently small, then for any $u \in \chi_{[E-e,E+e]}(H)\mathcal{H}$*

$$\lim_{t\to\infty}\big\langle \mathrm{e}^{-\mathrm{i}tH}u, (I - Q_4)\mathrm{e}^{-\mathrm{i}tH}u\big\rangle = 0.$$

Proof. *Step* 1. Set $\chi = \chi_{-,N,2N}$. We first prove

$$\lim_{N\to\infty}\limsup_{t\geqslant 1}\big\langle \mathrm{e}^{-\mathrm{i}tH}u, \big(I - \chi\big(r^2/t^2\big)\big)\mathrm{e}^{-\mathrm{i}tH}u\big\rangle = 0. \tag{4.32}$$

For that it suffices to show that there exist $\delta' > 0$ and $R \in \mathcal{B}(\mathcal{H})$ such that

$$\|R\| \leqslant Ct^{-1-\delta'} \quad \text{uniformly in } N \geqslant 1, \tag{4.33a}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\big\langle \mathrm{e}^{-\mathrm{i}tH}u, \big(I - \chi\big(r^2/t^2\big)\big)\mathrm{e}^{-\mathrm{i}tH}u\big\rangle \leqslant \langle u, Ru\rangle. \tag{4.33b}$$

We calculate, cf. (1.13) and (4.16),

$$\mathrm{D}_H\chi\big(r^2/t^2\big)=\begin{cases}\frac{r}{t^2}\chi'(r^2/t^2)(p_r-r/t)+\text{h.c.},\\ \frac{r}{t^2}\chi'(r^2/t^2)(\nabla r)_i g^{ij}(p-\nabla K)_j+\text{h.c.}\end{cases} \tag{4.34}$$

We will now use the first identity in (4.34). (For the second identity we use implicitly that t is large.) Clearly there is here the positive term $-2\frac{r^2}{t^3}\chi'(r^2/t^2)$ which for t large is equal to $2\frac{r}{t^2}\tilde\chi^2(r/t)$ where $\tilde\chi(s)=\sqrt{-|s|\chi'(s^2)}$. The remaining term is symmetrized as

$$\frac{r}{t^2}\chi'\big(r^2/t^2\big)p_r+\text{h.c.}=-t^{-1}\tilde\chi(r/t)\big(p_r+p_r^*\big)\tilde\chi(r/t). \tag{4.35}$$

Next we use (4.8c) with $\chi=1$

$$\|p_rQ_3\|,\ \big\|Q_3p_r^*\big\|\leqslant C=\sqrt{2\|Q_3H_0Q_3\|},$$

yielding the lower bound

$$\begin{aligned}&\frac{r}{t^2}\chi'\big(r^2/t^2\big)(p_r-r/t)+\text{h.c.}\\&\quad\geqslant 2(\sqrt{N}-C)t^{-1}\tilde\chi^2(r/t)-t^{-1}\tilde\chi(r/t)\big(p_r(I-Q_3)+(I-Q_3)p_r^*\big)\tilde\chi(r/t).\end{aligned}$$

Due to Lemma 4.8 the second term to the right contributes to (4.33b) by a term whose norm is bounded by $CN^{-1}t^{-2}$. Whence for $N\geqslant C^2$ indeed we obtain (4.33a) and (4.33b) with $\delta'=1$.

Due to Step 1 it suffices to show that for any fixed N

$$\lim_{t\to\infty}\big\langle \mathrm{e}^{-\mathrm{i}tH}u,\psi\big(r^2/t^2\big)\mathrm{e}^{-\mathrm{i}tH}u\big\rangle=0, \tag{4.36}$$

where $\psi=\chi_{2E_1,2E_2,N,2N}$. For that we need two more steps.

Step 2. We prove that

$$\int_1^\infty\big\langle \mathrm{e}^{-\mathrm{i}tH}u,\psi\big(r^2/t^2\big)\mathrm{e}^{-\mathrm{i}tH}u\big\rangle t^{-1}\,\mathrm{d}t<\infty. \tag{4.37}$$

Put

$$\chi(s)=\int_{-\infty}^s\psi\big(\beta^2\big)\,\mathrm{d}\beta,$$

and compute, cf. (4.16), (4.34) and (4.35),

$$\begin{aligned}&\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{e}^{\mathrm{i}tH}\chi(r/t)\mathrm{e}^{-\mathrm{i}tH}\\&\quad=\frac{1}{2t}\mathrm{e}^{\mathrm{i}tH}\psi\big(r^2/t^2\big)^{1/2}\big((p_r-r/t)+\text{h.c.}\big)\psi\big(r^2/t^2\big)^{1/2}\mathrm{e}^{-\mathrm{i}tH}\\&\quad\leqslant\frac{1}{t}\mathrm{e}^{\mathrm{i}tH}\psi\big(r^2/t^2\big)^{1/2}(\operatorname{Re}p_r-\sqrt{2E_1})\psi\big(r^2/t^2\big)^{1/2}\mathrm{e}^{-\mathrm{i}tH}.\end{aligned}$$

Next to treat the contribution from $\operatorname{Re} p_r$ we proceed again as in Step 1 inserting factors of Q_3, and using (in the first estimation) that by (4.8c)

$$\operatorname{Re} p_r \leqslant \epsilon/2 + \epsilon^{-1} H_0 \quad \text{for all } \epsilon > 0,$$

$$\begin{aligned}
&\frac{1}{t} \mathrm{e}^{\mathrm{i}tH} \psi\big(r^2/t^2\big)^{1/2} \operatorname{Re} p_r \psi\big(r^2/t^2\big)^{1/2} \mathrm{e}^{-\mathrm{i}tH} \\
&\quad = \frac{1}{t} \mathrm{e}^{\mathrm{i}tH} \psi\big(r^2/t^2\big)^{1/2} Q_3 \operatorname{Re} p_r Q_3 \psi\big(r^2/t^2\big)^{1/2} \mathrm{e}^{-\mathrm{i}tH} + \text{remainder} \\
&\quad \leqslant \frac{1}{t} \mathrm{e}^{\mathrm{i}tH} \psi\big(r^2/t^2\big)^{1/2} Q_3 \big(\epsilon/2 + \epsilon^{-1}(H - V)\big) Q_3 \psi\big(r^2/t^2\big)^{1/2} \mathrm{e}^{-\mathrm{i}tH} + \text{remainder} \\
&\quad \leqslant \frac{1}{t} \mathrm{e}^{\mathrm{i}tH} \psi\big(r^2/t^2\big)^{1/2} Q_3 \big(\epsilon/2 + \epsilon^{-1}(E + 2e - V)\big) Q_3 \psi\big(r^2/t^2\big)^{1/2} \mathrm{e}^{-\mathrm{i}tH} + \text{remainder} \\
&\quad \leqslant \frac{1}{t} \big(\epsilon/2 + \epsilon^{-1}(E + 2e)\big) \mathrm{e}^{\mathrm{i}tH} \psi\big(r^2/t^2\big) \mathrm{e}^{-\mathrm{i}tH} + \text{remainder.}
\end{aligned}$$

The remainders are treated by Lemma 4.8 and Condition 1.4. They have norms bounded by Ct^{-2}. Taking $\epsilon = \sqrt{2(E+e)}$ we thus obtain

$$\begin{aligned}
&\frac{\mathrm{d}}{\mathrm{d}t} \chi_{[E-e,E+e]}(H) \mathrm{e}^{\mathrm{i}tH} \chi(r/t) \mathrm{e}^{-\mathrm{i}tH} \chi_{[E-e,E+e]}(H) \\
&\quad \leqslant -\frac{c}{t} \chi_{[E-e,E+e]}(H) \mathrm{e}^{\mathrm{i}tH} \psi\big(r^2/t^2\big) \mathrm{e}^{-\mathrm{i}tH} \chi_{[E-e,E+e]}(H) + O\big(t^{-2}\big); \\
&c = \sqrt{2E_1} - \sqrt{2(E+2e)}.
\end{aligned}$$

For $e > 0$ small enough the constant $c > 0$. Then (4.37) follows by integration and by using that χ is bounded.

Step 3. We prove (4.36). By (4.37) there exists a sequence $t_n \to \infty$ such that

$$\big\langle \mathrm{e}^{-\mathrm{i}t_n H} u, \psi\big(r^2/t_n^2\big) \mathrm{e}^{-\mathrm{i}t_n H} u \big\rangle \to 0.$$

Thus it suffices to show that

$$\int_1^\infty \left| \frac{\mathrm{d}}{\mathrm{d}t} \big\langle \mathrm{e}^{-\mathrm{i}tH} u, \psi\big(r^2/t^2\big) \mathrm{e}^{-\mathrm{i}tH} u \big\rangle \right| \mathrm{d}t < \infty. \tag{4.38}$$

But by calculations and estimations like in Step 2 we obtain that

$$\left| \frac{\mathrm{d}}{\mathrm{d}t} \big\langle \mathrm{e}^{-\mathrm{i}tH} u, \psi\big(r^2/t^2\big) \mathrm{e}^{-\mathrm{i}tH} u \big\rangle \right| \leqslant \frac{C}{t} \big\langle \mathrm{e}^{-\mathrm{i}tH} u, \big|\psi'\big(r^2/t^2\big)\big| \mathrm{e}^{-\mathrm{i}tH} u \big\rangle + \frac{C}{t^2} \|u\|^2. \tag{4.39}$$

We fix a non-negative function $\tilde\psi \in C_{\mathrm{c}}^\infty((E + E_1, \infty))$ with $\tilde\psi \psi' = \psi'$. By using Step 2 to this function (instead of ψ) we obtain (4.37) with ψ replaced $\tilde\psi$ (possibly by taking $e > 0$ smaller). Combining this bound with (4.39) we obtain (4.38), and hence the lemma follows. □

Corollary 4.14. *For all $u \in \chi_{[E-e,E+e]}(H)\mathcal{H}$ with $e > 0$ taken sufficiently small the bound* (3.6b) *holds.*

Next we shall show a version of the key phase space propagation estimate of [12,26] using here the quantities enlisted before (3.6a)–(3.6c).

Lemma 4.15. *For all $u \in \chi_{[E-e,E+e]}(H)\mathcal{H}$ and $\chi \in C_c^\infty(\mathbb{R}_+)$:*

$$\int_1^\infty \langle \chi(r/t)\mathrm{e}^{-\mathrm{i}tH}u, W^{1/2}\chi(r/t)\mathrm{e}^{-\mathrm{i}tH}u\rangle t^{-1}\,\mathrm{d}t < \infty. \tag{4.40}$$

Proof. Let $u \in \chi_e(H)\mathcal{H}$. Here and henceforth we abbreviate $\chi_e(H) = \chi_{[E-e,E+e]}(H)$. Let $\chi \in C_c^\infty(\mathbb{R}_+)$ and choose $\hat{\chi} \in C_c^\infty(\mathbb{R}_+)$ with $\hat{\chi} = 1$ on the support of χ. Possibly by enlarging $E_1 < E_2$ we can assume that $\hat{\chi}(r/t) = \hat{\chi}(r/t)Q_4$. We are going to use the conclusion of Corollary 4.14 for this Q_4. Note here that such "enlargement" is doable uniformly in the small parameter $e > 0$.

Step 1. We show that for any $\epsilon \in (0,1)$

$$\int_1^\infty \bigl|\bigl\langle (p_i - \partial_i K)Q_4\mathrm{e}^{-\mathrm{i}tH}u, f'\bigl(t^{2\epsilon-2}r^2\bigr)\bigl(\nabla^2 r^2\bigr)^{ij}(p_j - \partial_j K)Q_4\mathrm{e}^{-\mathrm{i}tH}u\bigr\rangle\bigr| t^{-1}\,\mathrm{d}t < \infty. \tag{4.41}$$

We shall use the family of observables $\chi_e(H)Q_4\tilde{G}Q_4\chi_e(H)$. Clearly this family is bounded. We calculate the Heisenberg derivative. For the leading term coming from the derivative of $\tilde{G}$ we invoke Lemmas 4.5 and 4.8 yielding

$$\begin{aligned}&\chi_e(H)Q_4(\mathrm{D}_H\tilde{G})Q_4\chi_e(H)\\ &\quad\geqslant \frac{1}{2t}\chi_e(H)Q_4(p_i - \partial_i K)^* f'(\cdot)\bigl(\nabla^2 r^2\bigr)^{ij}(p_j - \partial_j K)Q_4\chi_e(H) + O\bigl(t^{-\epsilon'-1}\bigr).\end{aligned}$$

Combining this estimate with

$$\int_1^\infty \bigl|\mathrm{Re}\bigl\langle(\mathrm{D}_H Q_4)\mathrm{e}^{-\mathrm{i}tH}u, \tilde{G}Q_4\mathrm{e}^{-\mathrm{i}tH}u\bigr\rangle\bigr|\mathrm{d}t < \infty, \tag{4.42}$$

we obtain (4.41) by integration. In turn (4.42) follows using first that

$$\chi_e(H)(\mathrm{D}_H Q_4)\tilde{G}Q_4\chi_e(H) + \text{ h.c. } = \chi_e(H)\,\mathrm{Re}\bigl(\bigl(\mathrm{D}_H Q_4^2\bigr)\tilde{G}\bigr)\chi_e(H) + O\bigl(t^{-2}\bigr),$$

and then invoking (4.34) and Lemma 4.8 to rewrite the first term as

$$\chi_e(H)\,\mathrm{Re}\bigl(\bigl(\mathrm{D}_H Q_4^2\bigr)\tilde{G}\bigr)\chi_e(H) = t^{-1}\chi_e(H)\,\mathrm{Re}\bigl(\tilde{\chi}'(r/t)B\bigr)\chi_e(H) + O\bigl(t^{-3/2-\kappa}\bigr)$$

with $\tilde{\chi}(s) = \chi^2_{-,2E_1,2E_2}(s^2)$ and $B = B(t)$ being uniformly bounded. Using (4.15a) again we also conclude that

$$-\operatorname{Re}\big(\tilde\chi'(\cdot)B\big)=\sqrt{\big|\tilde\chi'\big|(\cdot)}\operatorname{Re}(B)\sqrt{\big|\tilde\chi'\big|(\cdot)}+O\big(t^{-1}\big). \tag{4.43}$$

Whence the contribution from the first term in (4.43) can be treated by using (3.6b) while the contribution from the second term as well as previous error terms clearly are integrable.

Step 2. We show (4.40). From (4.41) we can deduce the estimate

$$\int_1^\infty \big\langle \chi(r/t)\mathrm{e}^{-\mathrm{i}tH}u, W\chi(r/t)\mathrm{e}^{-\mathrm{i}tH}u\big\rangle t^{-1}\,\mathrm{d}t<\infty. \tag{4.44}$$

This estimate also holds with $\chi\to\hat\chi$. The proof goes as follows: First we estimate (using commutation)

$$\begin{aligned}
&\big\|\sqrt{W}\chi(r/t)\mathrm{e}^{-\mathrm{i}tH}u\big\|^2\\
&\quad=\big\|\sqrt{W}\chi(r/t)Q_4\mathrm{e}^{-\mathrm{i}tH}u\big\|^2\\
&\quad\leqslant\big\langle(p_i-\partial_iK)Q_4\mathrm{e}^{-\mathrm{i}tH}u,\chi(r/t)^2g^{ij}(p_j-\partial_jK)Q_4\mathrm{e}^{-\mathrm{i}tH}u\big\rangle+Ct^{-1}\|u\|^2\\
&\quad\leqslant\big(\sup|\chi|^2\big)\big\|f'\big(t^{2\epsilon-2}r^2\big)^{1/2}(p-\nabla K)Q_4\mathrm{e}^{-\mathrm{i}tH}u\big\|^2+t^{-1}C\|u\|^2.
\end{aligned}$$

Due to Condition 1.2 and (4.41) we have for a large $t_0\geqslant 1$

$$\begin{aligned}
&\int_1^\infty\big\|f'\big(t^{2\epsilon-2}r^2\big)^{1/2}(p-\nabla K)Q_4\mathrm{e}^{-\mathrm{i}tH}u\big\|^2t^{-1}\,\mathrm{d}t\\
&\quad\leqslant\int_1^{t_0}\big\|f'\big(t^{2\epsilon-2}r^2\big)^{1/2}(p-\nabla K)Q_4\mathrm{e}^{-\mathrm{i}tH}u\big\|^2t^{-1}\,\mathrm{d}t\\
&\qquad+(1+\delta)^{-1}\int_{t_0}^\infty\big\langle(p_i-\partial_iK)Q_4\mathrm{e}^{-\mathrm{i}tH}u,f'\big(t^{2\epsilon-2}r^2\big)\big(\nabla^2r^2\big)^{ij}(p_j-\partial_jK)Q_4\mathrm{e}^{-\mathrm{i}tH}u\big\rangle t^{-1}\,\mathrm{d}t\\
&\quad<\infty,
\end{aligned}$$

showing then (4.44).

Consider now the uniformly bounded observables (cf. (4.50) given below)

$$B^*\sqrt{W+t^{-\sigma}}B;\quad B:=\chi(r/t)\chi_e(H)\text{ and }\sigma\in(0,2).$$

We use (3.9) to write

$$\sqrt{W+t^{-\sigma}}=\pi^{-1}\int_0^\infty s^{-1/2}\big(W+t^{-\sigma}+s\big)^{-1}\big(W+t^{-\sigma}\big)\,\mathrm{d}s, \tag{4.45}$$

and then in turn calculate

$$\mathrm{D}_{H_0}\sqrt{W+t^{-\sigma}}=\pi^{-1}\int_0^\infty s^{1/2}\big(W+t^{-\sigma}+s\big)^{-1}\big((\mathrm{D}_{H_0}W)-\sigma t^{-\sigma-1}\big)\big(W+t^{-\sigma}+s\big)^{-1}\,\mathrm{d}s.$$

Next we apply Corollary 4.3 and use the Cauchy Schwarz inequality as in the proof of Lemma 4.11. This leads to the following bound for any $r_1>r_0$ and suitable constants $c, C>0$:

$$\begin{aligned}&B^*\big(\mathrm{D}_{H_0}\sqrt{W+t^{-\sigma}}\big)B\\&\quad\leqslant -\frac{c}{t}B^*W^{1/2}B+\frac{C}{t}\int_0^\infty s^{1/2}B^*\big(W+t^{-\sigma}+s\big)^{-1}\\&\qquad\times\big[(p_i-\partial_iK)^*\chi_{-,r_0,r_1}(r)g^{ij}(p_j-\partial_jK)+t^2|\tilde\gamma|^2\big]\big(W+t^{-\sigma}+s\big)^{-1}B\,\mathrm{d}s.\end{aligned}\tag{4.46}$$

Next we note that (minus) the integral of the first term is the quantity that enters in (4.40), so it suffices to show that the contribution from the second term is integrable as well as to show the bounds

$$\int_1^\infty \big\|B^*V\sqrt{W+t^{-\sigma}}B\big\|\,\mathrm{d}t<\infty,\tag{4.47a}$$

$$\int_1^\infty \big|\big\langle\big(\mathrm{D}_{H_0}\chi(r/t)\big)\mathrm{e}^{-\mathrm{i}tH}u,\sqrt{W+t^{-\sigma}}\chi(r/t)\mathrm{e}^{-\mathrm{i}tH}u\big\rangle\big|\,\mathrm{d}t<\infty.\tag{4.47b}$$

As for the contribution from the second term in the square bracket in (4.46) we estimate using Lemma 4.6 with $d>c>0$ chosen to the left of the support of χ, $\epsilon>0$ such that $2-2\epsilon=\sigma$ and $N=N(s,t)\geqslant 1$ such that $Nt^{-\sigma}=t^{-\sigma}+s$

$$\begin{aligned}&\int_0^\infty s^{1/2}\big\|B^*\big(W+t^{-\sigma}+s\big)^{-1}t^2|\tilde\gamma|^2\chi_{-,c,d}(r/t)\big(W+t^{-\sigma}+s\big)^{-1}B\big\|\,\mathrm{d}s\\&\quad\leqslant C_nt^{-\epsilon n}\int_0^\infty s^{1/2}\big(t^{-\sigma}+s\big)^{-2}\,\mathrm{d}s\\&\quad=\tilde C_nt^{\sigma/2-\epsilon n}.\end{aligned}\tag{4.48}$$

Choosing $n\in\mathbb{N}$ large enough gives integrability in t of this contribution. Similarly

$$\begin{aligned}&\int_0^\infty s^{1/2}\big\|B^*\big(W+t^{-\sigma}+s\big)^{-1}t^2|\tilde\gamma|^2\chi_{c,d,+}(r/t)\big(W+t^{-\sigma}+s\big)^{-1}B\big\|\,\mathrm{d}s\\&\quad\leqslant Ct^{-1-2\kappa}\int_0^\infty s^{1/2}\big(t^{-\sigma}+s\big)^{-2}\,\mathrm{d}s\\&\quad=\tilde Ct^{\sigma/2-1-2\kappa},\end{aligned}$$

yielding integrability in t of this contribution. As for the contribution from the first term in the square bracket in (4.46) we decompose

$$(p_i - \partial_i K)^* \chi_{-,r_0,r_1}(r) g^{ij}(p_j - \partial_j K) = 2W\chi_{-,r_0,r_1}(r) + \mathrm{i}(p_i - \partial_i K)^* g^{ij}(\partial_j r)\chi'_{-,r_0,r_1}(r).$$

In combination with the factor $(W + t^{-\sigma} + s)^{-1}$ to the left we thus obtain the uniform bound

$$\begin{aligned}&\big(W + t^{-\sigma} + s\big)^{-1}(p_i - \partial_i K)^* \chi_{-,r_0,r_1}(r) g^{ij}(p_j - \partial_j K)\\&\quad = O_{\mathcal{B}(\mathcal{H})}(1)\chi_{-,r_0,r_1}(r) + O_{\mathcal{B}(\mathcal{H})}\big(\big(t^{-\sigma} + s\big)^{-1/2}\big)\chi'_{-,r_0,r_1}(r).\end{aligned}$$

Next we note that it suffices to consider integrability in $t \in [t_0, \infty)$ for any sufficiently large $t_0 \geqslant 1$ (rather than in $t \in [1, \infty)$). We pick t_0 such that we can freely insert the above factor $\chi_{-,c,d}(r/t)$ to the right (for example $t_0 = \max(r_1/c, 1)$). Once this factor is inserted we invoke again Lemma 4.6 with ϵ and N chosen as above. We thus obtain for any $n \geqslant 0$

$$\big\|\chi_{-,c,d}(r/t)\big(W + t^{-\sigma} + s\big)^{-1} B\big\| \leqslant C_n t^{-n}\big(t^{-\sigma} + s\big)^{-n/2-1},$$

and to conclude we need to estimate (for some n)

$$\int_{t_0}^{\infty} \mathrm{d}t \int_0^{\infty} s^{1/2} t^{-n-1+\sigma/2}\big(t^{-\sigma} + s\big)^{-n/2-1}\, \mathrm{d}s < \infty. \tag{4.49}$$

Indeed (4.49) is true for any $n > 1$.

So we are left with proving (4.47a) and (4.47b). As for (4.47a) we note that $\|B^* V\| = O(t^{-1-\eta})$, hence integrable, and that

$$\begin{aligned}\big\|\sqrt{W + t^{-\sigma}}B\big\|^2 &\leqslant \big\|B^* W B\big\| + C_1 \leqslant \big\|B^*\big(2H_0 + |\nabla K|^2\big)B\big\| + C_1\\&\leqslant 2\big\|B^* H B\big\| + C_2 \leqslant C_3,\end{aligned} \tag{4.50}$$

where we in the last step used Lemma 4.8.

As for (4.47b) we write

$$\mathrm{D}_{H_0}\chi(r/t) = t^{-1}\operatorname{Re}\gamma; \quad \gamma := \chi'(r/t)(p_r - r/t).$$

We have, cf. (1.6b) and (4.8a),

$$\operatorname{Re}\gamma = \gamma + O\big(t^{-1/2-\kappa}\big).$$

Whence using the Cauchy Schwarz inequality we can estimate

$$\begin{aligned}
&\bigl|\bigl\langle\bigl(\mathrm{D}_{H_0}\chi(r/t)\bigr)\mathrm{e}^{-\mathrm{i}tH}u, \sqrt{W+t^{-\sigma}}\chi(r/t)\mathrm{e}^{-\mathrm{i}tH}u\bigr\rangle\bigr| \\
&\quad\leqslant t^{-1}\bigl(\bigl\|\gamma\mathrm{e}^{-\mathrm{i}tH}u\bigr\| + Ct^{-1/2-\kappa}\|u\|\bigr)\bigl\|\sqrt{W+t^{-\sigma}}B\mathrm{e}^{-\mathrm{i}tH}u\bigr\| \\
&\quad\leqslant C_1t^{-1}\bigl(\bigl\|\sqrt{W}\hat{\chi}(r/t)\mathrm{e}^{-\mathrm{i}tH}u\bigr\| + t^{-1/2-\kappa}\bigr)\bigl\|\sqrt{W+t^{-\sigma}}B\mathrm{e}^{-\mathrm{i}tH}u\bigr\| \\
&\quad\leqslant C_1t^{-1}\bigl\|\sqrt{W}\hat{\chi}(r/t)\mathrm{e}^{-\mathrm{i}tH}u\bigr\| \times \bigl\|\sqrt{W+t^{-\sigma}}B\mathrm{e}^{-\mathrm{i}tH}u\bigr\| + C_2t^{-3/2-\kappa} \\
&\quad\leqslant \frac{C_1}{2t}\bigl(\bigl\|\sqrt{W}\hat{\chi}(r/t)\mathrm{e}^{-\mathrm{i}tH}u\bigr\|^2 + \bigl\|\sqrt{W}B\mathrm{e}^{-\mathrm{i}tH}u\bigr\|^2\bigr) + C_3t^{-1-\sigma} + C_2t^{-3/2-\kappa}.
\end{aligned}$$

It remains to apply the bound (4.44) with χ as well as with $\chi \to \hat{\chi}$. □

The following type of result is called a *minimal velocity bound* in the literature.

Lemma 4.16. *For all $u \in \chi_{[E-e,E+e]}(H)\mathcal{H}$ with $e > 0$ taken sufficiently small the bound (3.6c) holds.*

Proof. Let $\chi \in C^\infty(\mathbb{R})$ be given such that $\chi' \in C_{\mathrm{c}}^\infty(\mathbb{R}_+)$ and the number $\sqrt{(1+\delta_2)^2E/2}$ is to the right of the support of χ. Then we shall show that

$$\int_1^\infty \bigl\|\chi(r/t)\mathrm{e}^{-\mathrm{i}tH}u\bigr\|^2 t^{-1}\,\mathrm{d}t < \infty, \tag{4.51}$$

showing in particular (3.6c).

Consider the following uniformly bounded observables

$$t^{-1}B^*AB; \quad B := \chi(r/t)\chi_e(H) \text{ and } A \text{ is given by (1.8}c\text{)}.$$

Due to Lemmas 4.8 and 4.12, for all sufficiently small $e > 0$

$$t^{-1}B^*(\mathrm{D}_HA)B \geqslant 2(1+\delta_1)Et^{-1}B^*B + O\bigl(t^{-3}\bigr).$$

Next, using this bound, Lemma 4.8 again and an estimation of the momentum in terms of the energy as in the proof of Lemma 4.13, we deduce

$$B^*\left(\mathrm{D}_H\frac{A}{t}\right)B = t^{-1}B^*(\mathrm{D}_HA)B - t^{-2}B^*AB \geqslant ct^{-1}B^*B + O\bigl(t^{-2}\bigr);$$
$$c = 2\bigl((1+\delta_1) - (1+\delta_2)\sqrt{1+2e/E}\bigr)E.$$

Here $c > 0$ for $e > 0$ small enough.

To complete the proof of the lemma it suffices to bound

$$\int_1^\infty \bigl|\mathrm{Re}\bigl\langle\bigl(\mathrm{D}_{H_0}\chi(r/t)\bigr)\mathrm{e}^{-\mathrm{i}tH}u, A\chi(r/t)\mathrm{e}^{-\mathrm{i}tH}u\bigr\rangle\bigr|t^{-1}\,\mathrm{d}t < \infty. \tag{4.52}$$

For that we also introduce $T := t^{-1}A\chi(r/t)Q_3$ and use (4.16), Lemma 4.8 and notation of Lemma 4.4 to write, with $\hat{\chi} \in C_c^\infty(\mathbb{R}_+)$ chosen such that $\hat{\chi} = 1$ on the support of χ,

$$\begin{aligned}&\langle (D_{H_0}\chi(r/t))e^{-itH}u, A\chi(r/t)e^{-itH}u\rangle \\ &\quad = \langle (\operatorname{Re} p_{\chi'(r/t)} - r/t\chi'(r/t))\hat{\chi}(r/t)e^{-itH}u, T\hat{\chi}(r/t)e^{-itH}u\rangle + O(t^{-1/2-\kappa}).\end{aligned}$$

Although it is here legitimate to replace $\operatorname{Re} p_{\chi'}$ by $p_{\chi'}$ and A by $(\partial_i r^2)g^{ij}p_j$ it is preferable to keep the symmetrized form. First we note that the energy localization (implemented by the appearance of the factor Q_3) makes $\|T\|$ uniformly bounded. We claim that for any $\sigma \in (0, 1+2\kappa]$ also the operators

$$S := (W + t^{-\sigma})^{-1/4}\operatorname{Re}(T^*(\operatorname{Re} p_{\chi'} - r/t\chi'))(W + t^{-\sigma})^{-1/4}$$

have uniformly bounded norm. Given this property we can bound the integral (4.52) by

$$\int_1^\infty |\langle (W + t^{-\sigma})^{1/4}\hat{\chi}(r/t)e^{-itH}u, S(W + t^{-\sigma})^{1/4}\hat{\chi}(r/t)e^{-itH}u\rangle| t^{-1}\,dt + C,$$

and we conclude by invoking Lemma 4.15. To bound S we note that interpolation yields

$$\|S\| \leqslant \|\operatorname{Re}(T^*(\operatorname{Re} p_{\chi'} - r/t\chi'))(W + t^{-\sigma})^{-1/2}\|,$$

and due to Lemma 4.9 we can write

$$\operatorname{Re}(T^*(\operatorname{Re} p_{\chi'} - r/t\chi')) = T^*\chi'(r/t)(p_r - r/t) + O(t^{-1/2-\kappa}).$$

Whence, using here also (4.8c), it follows that

$$\|S\| \leqslant \|T^*\| \times \|\chi'(r/t)(p_r - r/t)(W + t^{-\sigma})^{-1/2}\| + C_1 t^{\sigma/2-1/2-\kappa} \leqslant C_2. \qquad \square$$

Corollary 4.17. *For all $u \in \chi_{[E-e,E+e]}(H)\mathcal{H}$ with $e > 0$ taken sufficiently small (3.6a) holds.*

Proof. We use Lemma 4.13, Corollary 4.14, (4.51) and the subsequence argument in Step 3 in the proof of Lemma 4.13. Indeed there exists a sequence $t_n \to \infty$ such that

$$\lim_{n\to\infty} q(t_n) = 0; \quad q(t) := \langle e^{-itH}u, (I - Q_3Q_4Q_5^2Q_4Q_3)e^{-itH}u\rangle,$$

and the time-derivative of q is integrable due to Corollary 4.14 and (4.51). $\square$

4.5. *Proof of Lemma 3.2*

We prove Lemma 3.2 alone the line of the proof of Lemma 3.1 using the properties (3.6a)–(3.6c). So let Q_{p} be the operator defined by (3.5), and let $e > 0$ be small enough. Then the property i) follows by mimicking the proof of Lemma 4.11 using (3.6a)–(3.6c). This amounts to showing for $u \in \chi_{[E-e,E+e]}(H)\mathcal{H}$ and for the same quantity $T_N = T_N(t)$ as before the existence of $R = R(t) \in \mathcal{B}(\mathcal{H})$ such that

$$\int_{t_0}^{\infty} \left|\left\langle \mathrm{e}^{-\mathrm{i}tH}u, R\mathrm{e}^{-\mathrm{i}tH}u\right\rangle\right| \mathrm{d}t = o\left(t_0^0\right) \quad \text{uniformly in } N \geqslant 1, \tag{4.53a}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\left\langle \mathrm{e}^{-\mathrm{i}tH}u, Q_4Q_5\left(I - T_N^{-1}\right)Q_5Q_4\mathrm{e}^{-\mathrm{i}tH}u\right\rangle \leqslant \left\langle \mathrm{e}^{-\mathrm{i}tH}u, R\mathrm{e}^{-\mathrm{i}tH}u\right\rangle. \tag{4.53b}$$

We compute the derivative in (4.53b). The contribution from $\mathrm{D}_H T_N^{-1} = \mathrm{D}_{H_0} T_N^{-1} + \mathrm{i}[V, T_N^{-1}]$ is treated as before (note the trivial bound $Q_5\mathrm{i}[V, T_N^{-1}]Q_5 = O(t^{-1-\eta})$). It remains to consider the contribution

$$2\,\mathrm{Re}\left\langle \mathrm{e}^{\mathrm{i}tH}u, (\mathrm{D}_H Q_4Q_5)\left(I - T_N^{-1}(t)\right)Q_5Q_4\mathrm{e}^{-\mathrm{i}tH}u\right\rangle.$$

For that we compute $\mathrm{D}_H Q_4Q_5 = (\mathrm{D}_H Q_4)Q_5 + Q_4\mathrm{D}_H Q_5$, invoke (4.34) and Lemmas 4.4 and 4.8, and use (3.6b) and (3.6c) to treat the contributions from $\mathrm{D}_H Q_4$ and $\mathrm{D}_H Q_5$, respectively. Note that here the implementation of (3.6b) and (3.6c) requires symmetrization. For that part we use also Corollary 4.7.

As for the property 3.2 we use again use the proof of Lemma 4.11. The contribution from $\mathrm{D}_H T_{N(t)}^{-1} = \mathrm{D}_{H_0} T_{N(t)}^{-1} + \mathrm{i}[V, T_{N(t)}^{-1}]$ does not need elaboration. As for the contribution from $\mathrm{D}_H Q_4Q_5$ we compute as above using (4.34). We claim that this contribution indeed is $O(t^{-1-\delta'})$ for $\delta' \leqslant (1+\delta_1)/2$, as may be seen by using the localization provided by the factor Q_6^2. Indeed due to Lemma 4.4 we can bound for any $\chi \in C_c^\infty(\mathbb{R}_+)$

$$\left\|\left(\chi(r/t)(p_r - r/t) + \mathrm{h.c.}\right)Q_6^2\right\| \leqslant Ct^{-1/2-\delta_1/2}.$$

The property iii) is proved by commuting as in the proof of Lemma 3.1 iii). Thus the lemma is proved. □

References

[1] J.M. Bouclet, Resolvent estimates for the Laplacian on asymptotically hyperbolic manifolds, Ann. Henri Poincaré 7 (3) (2006) 527–561.

[2] I. Chavel, Riemannian Geometry—A Modern Introduction, Cambridge Tracts in Math., vol. 108, Cambridge University Press, Cambridge, 1993.

[3] H.D. Cornean, I. Herbst, E. Skibsted, Spiraling attractors and quantum dynamics for a class of long-range magnetic fields, J. Funct. Anal. 247 (1) (2007) 1–94.

[4] H.D. Cornean, I. Herbst, E. Skibsted, private communication, 2006.

[5] J. Cruz, E. Skibsted, Global solutions to the eikonal equation, preprint, 2011.

[6] J. Dereziński, C. Gérard, Scattering Theory of Classical and Quantum N-Particle Systems, Texts Monogr. Phys., Springer, Berlin, 1997.

[7] J. Dereziński, C. Gérard, Long-range scattering in the position representation, J. Math. Phys. 38 (8) (1997) 3925–3942.
[8] H. Donnelly, Spectrum of the Laplacian on asymptotically Euclidean spaces, Michigan Math. J. 46 (1) (1999) 101–111.
[9] J. Faupin, J.S. Møller, E. Skibsted, Second order perturbation theory for embedded eigenvalues, Comm. Math. Phys. 306 (2011) 193–228.
[10] R.G. Froese, P.D. Hislop, Spectral analysis of second-order elliptic operators on noncompact manifolds, Duke Math. J. 58 (1) (1989) 103–129.
[11] V. Georgescu, C. Gérard, J.S. Møller, Commutators, C_0-semigroups and resolvent estimates, J. Funct. Anal. 216 (2004) 303–361.
[12] G.M. Graf, Asymptotic completeness for NN-body short-range quantum systems: a new proof, Comm. Math. Phys. 132 (1990) 73–101.
[13] R. Gulliver, I. Lasiecka, W. Littman, R. Triggiani, The case for differential geometry in the control of single and coupled PDEs: the structural acoustic chamber, in: Geometric Methods in Inverse Problems and PDE Control, in: IMA Vol. Math. Appl., vol. 137, Springer, New York, 2004, pp. 73–181.
[14] I. Herbst, E. Skibsted, Quantum scattering for potentials independent of $|\mathbf{x}|$: asymptotic completeness for high and low energies, Comm. Partial Differential Equations 29 (3–4) (2004) 547–610.
[15] K. Ito, S. Nakamura, Time-dependent scattering theory for Schrödinger operators on scattering manifolds, J. Lond. Math. Soc. 81 (3) (2010) 774–792.
[16] K. Ito, E. Skibsted, Absence of embedded eigenvalues for Riemannian Laplacians, preprint, 2011.
[17] J. Jost, Riemannian Geometry and Geometric Analysis, Universitext, Springer, Berlin, 2008.
[18] H. Kumura, On the essential spectrum of the Laplacian on complete manifolds, J. Math. Soc. Japan 49 (1) (1997) 1–14.
[19] H. Kumura, Behavior of the curvature at infinity and the structure of the spectrum of the Laplacian, Sūgaku 59 (2) (2007) 154–170 (in Japanese).
[20] R. Melrose, Spectral and scattering theory for the Laplacian on asymptotically Euclidean spaces, in: Spectral and Scattering Theory, in: Lect. Notes Pure Appl. Math., vol. 161, Dekker, New York, 1994, pp. 85–130.
[21] R. Melrose, M. Zworski, Scattering metrics and geodesic flow at infinity, Invent. Math. 124 (1–3) (1996) 389–436.
[22] J. Milnor, Morse Theory, Princeton University Press, Princeton, 1963.
[23] J.S. Møller, E. Skibsted, Spectral theory of time-periodic many-body systems, Adv. Math. 188 (2004) 137–221.
[24] É. Mourre, Absence of singular continuous spectrum for certain selfadjoint operators, Comm. Math. Phys. 78 (3) (1980/1981) 391–408.
[25] M. Reed, B. Simon, Methods of Modern Mathematical Physics, vols. I–IV, Academic Press, New York, 1972–1978.
[26] I.M. Sigal, A. Soffer, Long-range many-body scattering. Asymptotic clustering for Coulomb-type potentials, Invent. Math. 99 (1) (1990) 115–143.
[27] D. Yafaev, Wave operators for the Schrödinger operator, Teoret. Mat. Fiz. 45 (1980) 224–234.