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Scattering theory from a geometric view point

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This article is based on the author's recent joint work with Erik Skibsted [IS1].

1 Assumptions

We discuss the scattering theory on a manifold with ends. Let (M,g) be a connected and complete d-dimensional Riemannian manifold. The Schrödinger operator we consider is

$$H=H_0+V;\quad H_0=-\frac{1}{2}\triangle,$$

and the Hilbert space $\mathcal{H}=L^2(M)$. For any local coordinates x we can write

$$g=g_{ij}\,\mathrm{d}x^i\otimes \mathrm{d}x^j,$$

and then the Laplace-Beltrami operator $-\triangle$ is defined locally by

$$-\triangle=p_i^*g^{ij}p_j=(\det g)^{-1/2}p_i(\det g)^{1/2}g^{ij}p_j,$$

where $\det g=\det(g_{ij})$, $(g^{ij})=(g_{ij})^{-1}$ and $p_i=-\mathrm{i}\partial_i$. Since the Riemannian density on M is given locally by $(\det g)^{1/2}\mathrm{d}x^1\cdots \mathrm{d}x^d$, $p_i^*=(\det g)^{-1/2}p_i(\det g)^{1/2}$ is indeed the adjoint of p_i. Under the conditions below H is essentially self-adjoint on $C_c^\infty(M)$. We denote the self-adjoint extension also by H.

We first impose an *end structure* on M, cf. [K].

Condition 1.1 (End structure). There exists a relatively compact open set $O\Subset M$ with smooth boundary ∂O such that the exponential map restricted to outward normal vectors on ∂O:

$$\exp_O:=\exp|_{N^+\partial O}\colon N^+\partial O\to M$$

is diffeomorphic onto $E:=M\setminus\overline{O}$.

A component of E is called an *end*, and such M a *manifold with ends.*

It is straightforward to see there exists a function $r\in C^\infty(M)$ such that

$$r(x)=\mathrm{dist}(x,O),\quad x\in E.$$

The function r is not uniquely determined on O, but we fix one.

Before stating the remaining conditions it would be a good motivation to see a Mourre-type commutator computation in an explicit form. We define the conjugate operator A by

$$A = \mathrm{i}[H_0, r^2] = \frac{1}{2}\{(\partial_i r^2)g^{ij}p_j + p_i^* g^{ij}(\partial_j r^2)\}. \tag{1.1}$$

Then we have by Proposition 9.1

$$\mathrm{i}[H_0, A] = p_i^*(\nabla^2 r^2)^{ij}p_j + \frac{\mathrm{i}}{4}(\partial_i \Delta r^2)g^{ij}p_j - \frac{\mathrm{i}}{4}p_i^* g^{ij}(\partial_j \Delta r^2). \tag{1.2}$$

Here $\nabla^2 f \in \Gamma(T^*M \otimes T^*M)$, $f \in C^\infty(M)$, denotes the geometric Hessian, and in local coordinates

$$(\nabla^2 f)_{ij} = \partial_i\partial_j f - \Gamma_{ij}^k \partial_k f; \quad \Gamma_{ij}^k = \frac{1}{2}g^{kl}(\partial_i g_{lj} + \partial_j g_{li} - \partial_l g_{ij}). \tag{1.3}$$

Sub- and superscripts are related through the identification $TM \cong T^*M$ by the metric tensor g, e.g.,

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

Now we impose:

Condition 1.2 (Mourre type condition). There exist $\delta \in (0,1]$ and $r_0 \geq 0$ such that for $x \in E$ with $r(x) \geq r_0$

$$\nabla^2 r^2 \geq (1+\delta)g. \tag{1.4}$$

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

$$|\nabla \Delta r^2|^2 = g^{ij}(\partial_i \Delta r^2)(\partial_j \Delta r^2) \leq C\langle r\rangle^{-1-\kappa}. \tag{1.5}$$

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

$$|V(x)| \leq C\langle r\rangle^{-1-\eta}. \tag{1.6}$$

The inequality (1.4) is understood as that for quadratic forms on fibers of TM, and we have used the standard notation $\langle r\rangle = (1+r^2)^{1/2}$.

We call Condition 1.3 the quantum mechanics bound, because we do not have to assume Condition 1.3 in the analysis of the corresponding classical mechanics. See Section 6. In fact the quantities $\partial_i \Delta r^2$ appears only in the remainder terms in (1.2), so that they do not survive in the classical mechanics.

2 Free propagator

Our free propagator $U(t)$ is not e^{-itH_0}. Define $U(t)$, $t>0$, by

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

with $K(t,x) = r(x)^2/2t$ and A given by (1.1).

By the eikonal equation

$$|\nabla r|^2 = g^{ij}(\partial_i r)(\partial_j r) = 1 \quad \text{on } E$$

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

$$\partial_t K = -\frac{1}{2}g^{ij}(\partial_i K)(\partial_j K) \quad \text{on } E. \tag{2.1}$$

On the other hand, $e^{-i\frac{\ln t}{2}A}$ has an explicit representation

$$e^{-i\frac{\ln t}{2}A}u(x) = \exp\Big(\int_1^t \frac{1}{4s}(-\Delta r^2)(\omega(s,x))\,ds\Big)u(\omega(t,x)), \tag{2.2}$$

where the flow $\omega = \omega(t,x)$, $(t,x)\in(0,\infty)\times M$, is specified by

$$\partial_t\omega^i = -\frac{1}{2t}g^{ij}(\omega)(\partial_j r^2)(\omega), \quad \omega(1,x) = x. \tag{2.3}$$

In fact, the (time-dependent) generator of $e^{-i\frac{\ln t}{2}A}$ is a differential operator of first order, and we obtain (2.2) by solving the transport equation.

We note that $e^{-i\frac{\ln t}{2}A}$ is the geodesic dilation on $\mathcal{H}$ with respect to r. To see that we can compute, using the relation $-\Delta f = g^{ij}(\nabla^2 f)_{ij} = \operatorname{tr}(\nabla^2 f)$,

$$\exp\Big(\int_1^t \frac{1}{4s}(-\Delta r^2)(\omega(s,x))\,ds\Big) = J(\omega(t,x))^{1/2}\Big(\frac{\det g(\omega(t,x))}{\det g(x)}\Big)^{1/4}, \tag{2.4}$$

and note that (2.3) is solved for $(t,x)\in(0,\infty)\times E$ by

$$\omega(t,x) = \exp_O\Big[\frac{1}{t}(\exp_O)^{-1}(x)\Big],$$

(and for $(t,x)\in(0,\infty)\times O$ by something different and complicated). The first factor in the right-hand side of (2.4) is the Jacobian for $\omega(t,\cdot)$, and the second concerns the change of density for $\omega(t,\cdot)$.

Hence, in particular, $U(t)$ is unitary both on

$$\mathcal{H}_{\mathrm{aux}} := L^2(E)\subset\mathcal{H}, \quad (\mathcal{H}_{\mathrm{aux}})^\perp = L^2(O)\subset\mathcal{H}.$$

Remark 2.1. This type of the free propagator appeared first in [Y]. Refer to [DG, CHS, HS] for later developments. It would be possible to compare e^{-itH} with e^{-itH_0}, but e^{-itH_0} is something "we do not know very much" as well as e^{-itH}. We will see briefly why e^{-itH} is comparable with $U(t)$ by investigating the generators.

3 Generator of the free propagator

Let $G(t)$ be the time-dependent generator of $U(t)$:

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

By formal computation

$$\begin{aligned} G(t) &= -\partial_t K + \mathrm{e}^{iK}\frac{1}{2t}A\mathrm{e}^{-iK} \\ &= -\partial_t K + \frac{1}{2}\{(\partial_i K)g^{ij}(p_j - \partial_j K) + (p_i - \partial_i K)g^{ij}(\partial_j K)\}. \end{aligned}$$

Hence we can see

$$H - G(t) = V + W(t) + \alpha(t) \tag{3.1}$$

with

$$\begin{aligned} W(t) &= \frac{1}{2}(p_i - \partial_i K)^* g^{ij}(p_j - \partial_j K) = \mathrm{e}^{\mathrm{i}K}H_0\mathrm{e}^{-\mathrm{i}K}, \\ \alpha(t) &= \alpha(t,x) = (\partial_t K) + \frac{1}{2}g^{ij}(\partial_i K)(\partial_j K). \end{aligned}$$

The first and the third terms in (3.1) are short-range by Condition 1.4 and (2.1); For any $N > 0$

$$|\alpha(t,x)| \le C_N t^{-2}\langle r\rangle^{-N}.$$

Moreover, we may say from classical point of view, so is the second term $W(t)$; For any nontrapped classical trajectory $(x(t), p(t))$

$$0 \le \frac{1}{2}g^{ij}(x(t))\{p_i(t) - \partial_i K(t,x(t))\}\{p_j(t) - \partial_j K(t,x(t))\} \le C\langle t\rangle^{-1-\delta}, \tag{3.2}$$

cf. the fact that K is a solution to the Hamilton-Jacobi equation. In fact, the translation of the estimate (3.2) into the quantum mechanics is the heart of the proof of our main results.

We remark that, since

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

which we can see with ease in the *geodesic spherical coordinates*, $G(t)$ differs from the one-dimensional radial Laplacian by a short-range term. Note that $r(t)/t$ classically approaches the radial momentum $p_r(t)$, cf. (3.2). Hence we could choose the radial Laplacian as the free operator, see [IN] for a similar relationship.

4 Main results

We state the main results concerning the wave operator:

Theorem 4.1 (Wave operator). *Suppose Conditions 1.1–1.4. Then there exist the strong limits*

$$\Omega_+ := \operatorname*{s-lim}_{t\to+\infty} e^{itH}U(t)P_{\mathrm{aux}}, \quad \widetilde{\Omega}_+ := \operatorname*{s-lim}_{t\to+\infty} U(t)^* e^{-itH}P_{\mathrm{c}},$$

where P_{aux} and P_{c} are the projections onto $\mathcal{H}_{\mathrm{aux}}$ and $\mathcal{H}_{\mathrm{c}}(H)$, the continuous subspace for H, respectively. Moreover the wave operator Ω_+ is complete, i.e.

$$\widetilde{\Omega}_+ = \Omega_+^*, \quad \Omega_+^*\Omega_+ = P_{\mathrm{aux}}, \quad \Omega_+\Omega_+^* = P_{\mathrm{c}}.$$

We will not give the proof in detail in this article.

It would be proved in [IS2] that H would not have positive eigenvalues even with conditions slightly weakened, and then $\mathcal{H}_{\mathrm{c}}(H) = \chi_{(0,\infty)}(H)\mathcal{H}$. Here we have used the notation $\chi_{\mathcal{O}}$ to denote the characteristic function of $\mathcal{O} \subset \mathbb{R}$. It follows by a standard local compactness argument that the negative spectrum of H (if not empty) consists of eigenvalues of finite multiplicity accumulating at most at zero.

Corollary 4.2 (Intertwining property and spectrum). *One has the intertwining property:*

$$\Omega_+^* H \Omega_+ = \frac{1}{2} r^2 P_{\mathrm{aux}}.$$

In particular, the singular continuous spectrum of H is absent, i.e., $\sigma_{\mathrm{sc}}(H) = \varnothing$, and the continuous spectrum $\sigma_{\mathrm{c}}(H) = [0,\infty)$.

The following corollary implies the existence of "the asymptotic speed". For self-adjoint operators A and A_i, $i = 1, 2, \dots$, we denote

$$A = \operatorname*{s-}C_{\mathrm{c}}(\mathbb{R})\operatorname*{-lim}_{i\to+\infty} A_i,$$

if for any $f \in C_{\mathrm{c}}(\mathbb{R})$ the following equality holds:

$$f(A) = \operatorname*{s-lim}_{i\to+\infty} f(A_i).$$

Corollary 4.3 (Asymptotic observables). *In the continuous subspace $\mathcal{H}_{\mathrm{c}}(H)$ there exists the $*$-representation*

$$\omega_\infty^+ = \operatorname*{s-}C_{\mathrm{c}}(M)\operatorname*{-lim}_{t\to+\infty} e^{itH}\omega(t,\cdot)e^{-itH}. \tag{4.1}$$

In particular, the asymptotic speed

$$r(\omega_\infty^+) = \operatorname*{s-}C_{\mathrm{c}}(\mathbb{R})\operatorname*{-lim}_{t\to+\infty} e^{itH}\,\frac{r(\cdot)}{t}\,e^{-itH}$$

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

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

$$\varphi(\omega_\infty^+) = \Omega_+\varphi\Omega_+^*, \quad H_{\mathrm{c}} = 2^{-1}r(\omega_\infty^+)^2.$$

In local coordinates $\omega(t,\cdot)$ has d components which we can substitute for any $f \in C_c(M)$, so the limit in (4.1) makes sense.

Remarks 4.4. 1. The quantities appearing in the above argument are independent of choice of r on O.

2. Conditions 1.2–1.4 are optimal in the sense that we can construct counterexamples to the existence of Ω_+ under the slight relaxation of the conditions allowing either $\delta = 0$ in (1.4), $\kappa = 0$ in (1.5) or $\eta = 0$ in (1.6).

5 Example: Rotationally symmetric manifold

Here we look at only one example that tells us what type of ends are in the scope of Conditions 1.2 and 1.3 intrinsically.

First we note that Condition 1.1 ensure the existence of *geodesic spherical coordinates* $(r, \sigma) \in (0,\infty) \times \partial O$ on ends E, which are given by

$$r(x) = \mathrm{dist}\,(x, O) = |(\exp_O)^{-1}(x)|, \quad \sigma(x) = \pi \circ (\exp_O)^{-1}(x)$$

for $x \in E$. Then by Gauss's lemma we can write

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

where the Greek indices run on $2, \dots, d$.

Keeping this in mind, we let (M, g) be a complete Riemannian manifold such that $M \setminus \{o\} \cong (0,\infty) \times \mathbb{S}^{d-1}$ for some $o \in M$ and that with respect to coordinates $(r, \sigma) \in (0,\infty) \times \mathbb{S}^{d-1}$

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

Then Condition 1.1 is automatically satisfied. Due to a regularity consideration for g at o the tensor h has to be is the standard metric on the unit sphere and $\lim_{r\to 0} r^{-2}f(r) = 1$, but such consideration is not needed in the framework of Section 1.

Then, by (1.3), it follows

$$(\nabla^2 r^2)_{rr} = 2, \quad (\nabla^2 r^2)_{r\alpha} = (\nabla^2 r^2)_{\alpha r} = 0, \quad (\nabla^2 r^2)_{\alpha\beta} = rf' h_{\alpha\beta}.$$

Thus, if we set $f = \mathrm{e}^{2\varphi}$, (1.4) is equivalent to

$$2r\varphi' \ge 1 + \delta, \tag{5.1}$$

and, by $\triangle r^2 = g^{ij}(\nabla^2 r^2)_{ij} = 2 + 2(d-1)r\varphi'$, (1.5) to

$$|(r\varphi')'| \le C\langle r\rangle^{-(1+\kappa)/2}. \tag{5.2}$$

We see that the inequalities (5.1) and (5.2) allow, for example,

$$\begin{aligned} f(r) &= f_{1,\mu}(r) = r^2\langle r\rangle^{2\mu}, \quad \mu \ge -(1-\delta)/2, \\ f(r) &= f_{2,\nu}(r) = r^2\mathrm{e}^{-2}\exp(2\langle r\rangle^\nu), \quad 0 \le \nu \le (1-\kappa)/2. \end{aligned}$$

Note that the Euclidean space corresponds to $f(r) = f_{1,0}(r) = f_{2,0}(r) = r^2$.

6 Classical scattering

In this section we consider the corresponding classical scattering. We note that our proofs of Theorem 4.1 and Corollary 4.3 do not require but are strongly motivated by these classical mechanics considerations. As we pointed out before, the classical mechanics considerations only require Conditions 1.1 and 1.2.

6.1 Regularity of inverse dilation on ends

Recall that the flow $\omega = \omega(t, x)$, $(t, x) \in (0, \infty) \times M$, is defined by

$$\partial_t \omega^i = -\frac{1}{2t} g^{ij}(\omega)(\partial_j r^2)(\omega), \quad \omega(1, x) = x, \tag{6.1}$$

and, for $(t, x) \in (0, \infty) \times E$, written by

$$\omega(t, x) = \exp_O \Big[\frac{1}{t} (\exp_O)^{-1}(x) \Big].$$

Lemma 6.1. *For any $x \in E$ with $r(x) \geq r_0$ and $t \in (0, r(x)/r_0)$*

$$g^{ij}(x) g_{kl}(\omega(t, x))[\partial_i \omega^k(t, x)][\partial_j \omega^l(t, x)] \leq d t^{-(1+\delta)}. \tag{6.2}$$

Proof. We note that the left-hand side of (6.2) is independent of choice of coordinates. Fix $x \in E$ 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,

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

(The definition of $\nabla_{\partial_t \omega}$ is given below.) From (6.1) it follows that

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

Thus, taking summation in i, j, we obtain for $t \in (0, r/r_0)$

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

Noting $g^{ij}(x) g_{kl}(\omega)(\partial_i \omega^k)(\partial_j \omega^l)\big|_{t=1} = d$, we have (6.2). □

6.2 Mourre estimate

Set

$$h_0(x,p) = \frac{1}{2} g^{ij}(x) p_i p_j, \quad (x,p) \in T^*M.$$

Definition 6.2. The *classical trajectory* $(x(t), p(t)) \in T^*M$ is a solution to the Hamiltonian equation

$$\dot{x} = \frac{\partial h_0}{\partial p}, \quad \dot{p} = -\frac{\partial h_0}{\partial x}.$$

The classical trajectory $(x(t), p(t))$ is *forward nontrapped*, if there exists a sequence $t_n \to +\infty$ such that

$$\lim_{n \to +\infty} r(x(t_n)) = +\infty.$$

The following proposition is on the classical Mourre estimate:

Proposition 6.3. *For any classical trajectory $(x(t), p(t))$ the following estimate holds:*

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2} r(x(t))^2 \geq 2(1+\delta) h_0 \quad \textit{for } x(t) \in E \textit{ with } r(x(t)) \geq r_0.$$

In particular, if $(x(t), p(t))$ is forward nontrapped, there exists $C > 0$ such that

$$r(x(t)) \geq Ct - C. \tag{6.3}$$

Proof. The assertion follows from the fact that $x(t)$ satisfies the geodesics equation $\ddot{x}^i + \Gamma^i_{jk} \dot{x}^j \dot{x}^k = 0$. □

6.3 Propagation estimates

Set

$$w(t,x,p) = \frac{1}{2} g^{ij}(x)(p_i - \partial_i K(t,x))(p_j - \partial_j K(t,x)); \quad K(t,x) = \frac{r(x)^2}{2t},$$

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

Lemma 6.4. *For any forward nontrapped classical trajectory $(x(t), p(t))$ there exists $C > 0$ such that*

$$w(t, x(t), p(t)) \leq C t^{-(1+\delta)}. \tag{6.4}$$

Proof. We compute

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

By (2.1)

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

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

$$0 = \partial_k g^{ij} + \Gamma^i_{kl}g^{lj} + \Gamma^j_{kl}g^{il}, \tag{6.5}$$

so that

$$\partial_i g^{kl}(\partial_k K)(\partial_l K) = 2(\nabla^2 K)_{ik}g^{kl}(\partial_l K). \tag{6.6}$$

Thus

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

On the other hand, by (6.5) and (6.6) again we have

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

Hence, summing up and noting (6.3), we obtain for large t

$$\frac{\mathrm{d}}{\mathrm{d}t}w = -(p_l - \partial_l K)g^{lk}(\nabla^2 K)_{ki}g^{ij}(p_j - \partial_j K) \le -\frac{1+\delta}{t}w.$$

This implies (6.4). □

Proposition 6.5. *For any forward nontrapped $x(t)$ there exists the limit*

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

Proof. Due to the flow equation (6.1) we have the group property $\omega(t, \omega(s,x)) = \omega(ts, x)$. Hence it suffice to consider the trajectories with $C > r_0$ in (6.3). On the other hand, differentiate

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

in t, and use then (6.1) to obtain

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

Putting $s = 1$, we obtain

$$\partial_t \omega^i(t,x) = -g^{kl}(x)(\partial_k \omega^i)(t,x)(\partial_l K)(t,x). \tag{6.7}$$

By applying first (6.7), and then (6.2) and (6.4), we obtain

$$\begin{aligned} g_{ij}\dot{\omega}^i\dot{\omega}^j &= g_{ij}[\partial_t\omega^i + (\partial_p h_0)(\partial_x \omega^i)][\partial_t \omega^j + (\partial_p h_0)(\partial_x \omega^j)] \\ &= g_{ij} g^{kl}(\partial_k \omega^i)(p_l - \partial_l K) g^{mn}(\partial_m \omega^j)(p_n - \partial_n K) \\ &\leq C t^{-2(1+\delta)}, \end{aligned}$$

and the assertion follows. □

7 Reduction of proof of Theorem 4.1

In this section we reduce the proof to the construction of escaping functions $Q_{\mathrm{f}}(t)$ and $Q_{\mathrm{p}}(t)$ for the *free* and the *perturbed* dynamics, respectively.

For all practical purposes we consider (3.1) 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 section Theorem 4.1 is a consequence of the following two lemmas:

Lemma 7.1. *Let $0 < \mu < M < \infty$. Then there exists a weakly differentiable*

$$Q_{\mathrm{f}} \colon [1,\infty) \to \mathcal{B}_{\mathrm{sa}}(\mathcal{H})$$

such that $\|Q_{\mathrm{f}}(t)\|_{\mathcal{B}(\mathcal{H})} \leq 1$ and for some $\delta' > 0$

1.

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

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

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

3. The operator $(W(t) + \alpha(t) + V)Q_{\mathrm{f}}(t)$ is $O_{\mathcal{B}(\mathcal{H})}(t^{-1-\delta'})$.

Lemma 7.2. *Let $E \in (0,\infty)$, and $e > 0$ small. Then there exists a weakly differentiable*

$$Q_{\mathrm{p}} \colon [1,\infty) \to \mathcal{B}_{\mathrm{sa}}(\mathcal{H})$$

such that $\|Q_{\mathrm{p}}(t)\|_{\mathcal{B}(\mathcal{H})} \leq 1$ and for some $\delta' > 0$

1.

$$\operatorname*{s-lim}_{t\to\infty} (I - Q_{\mathrm{p}}(t)) \mathrm{e}^{-\mathrm{i}tH} \chi_{[E-e,E+e]}(H) P_{\mathrm{c}} = 0,$$

2. The operators $HQ_{\mathrm{p}}(t)$ and $Q_{\mathrm{p}}(t)H$ are bounded, and

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

3. The operator $(W(t) + \alpha(t) + V)Q_{\mathrm{p}}(t)$ is $O_{\mathcal{B}(\mathcal{H})}(t^{-1-\delta'})$.

Now we deduce Theorem 4.1 from Lemmas 7.1 and 7.2. The proof of the existence of Ω_+ and $\widetilde{\Omega}_+$ are completely the same and we discuss only Ω_+. From Lemma 7.1 2 and 3 the following statement follows, which combined with Lemma 7.1 1 and a density argument implies the existence of the wave operator.

Lemma 7.3. *Let $\mu, M, Q_{\mathrm{f}}, \delta'$ be as in Lemma 7.1, and $u \in \chi_{[\mu,M]}(r^2)\mathcal{H}_{\mathrm{aux}} \cap C^\infty(M)$. Then for any $\varepsilon > 0$ there exists $t_0 > 0$ such that for any $t, t' \geq t_0$ and $v \in C_c^\infty(M)$*

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

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

Proof. Let $\varepsilon > 0$. For any $t \geq t' \geq 1$ and $v \in C_c^\infty(M)$ we compute, using Lemma 7.1 2 and 3 and the Schwarz inequality,

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

By Lemma 7.1 3

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

so that

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

Similarly, we have

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

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

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

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

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

Thus the lemma follows. □

As for the limit $\widetilde{\Omega}_+$ the following lemma is sufficient. We omit the proof.

Lemma 7.4. *Let $E, e, Q_{\mathrm{p}}, \delta'$ be as in Lemma 7.2 and $u \in \chi_{[E-e,E+e]}(H) P_{\mathrm{c}}(C_{\mathrm{c}}^\infty(M))$. Then for any $\varepsilon > 0$ there exists $t_0 > 0$ such that for any $t, t' \geq t_0$ and $v \in C_{\mathrm{c}}^\infty(M)$*

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

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

8 Localization operators in explicit form

We give the explicit formulas for Q_{f} and Q_{p} that satisfy Lemmas 7.1 and 7.2.

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

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

and that

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

We also assume that the family of these cutoff functions satisfies

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

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

$$\begin{aligned} Q_{\mathrm{f}}(t) &= (Q_2(t) Q_1(t))^* Q_2(t) Q_1(t), \\ Q_{\mathrm{p}}(t) &= (Q_6(t) Q_5(t) Q_4(t))^* Q_6(t) Q_5(t) Q_4(t), \end{aligned}$$

where we use quantities from the list

$$\begin{aligned} Q_1(t) &= \chi_{\mu_1,\mu,M,M_1}\Big(\frac{r^2}{t^2}\Big), & Q_2(t) &= (I + t^{1+\delta_1} W(t))^{-1/2}, \\ Q_3 &= \chi_{E-2e,E-e,E+e,E+2e}(H), & Q_4(t) &= \chi_{-,2E_1,2E_2}\Big(\frac{r^2}{t^2}\Big), \\ Q_5(t) &= \chi_{(1+\delta_3)^2 E/2,(1+\delta_2)^2 E/2,+}\Big(\frac{r^2}{t^2}\Big), & Q_6(t) &= Q_2(t) = (I + t^{1+\delta_1} W(t))^{-1/2}. \end{aligned}$$

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

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

then Q_{f} satisfies Lemma 7.1. For given $E \in (0, \infty)$ let E_*, δ_* be any constants such that

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

and $e > 0$ small enough accordingly, then Q_{p} satisfies Lemma 7.2.

The operator functions Q_i, $i = 2, 3, 6$, are defined for instance as follows: Let T be a self-adjoint operator on a complex Hilbert space $\mathcal{H}$ and $\chi \in C_{\mathrm{c}}^\infty(\mathbb{R})$. We can choose an almost analytic extension $\tilde{\chi} \in C_{\mathrm{c}}^\infty(\mathbb{C})$, i.e.

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

Then the Helffer-Sjöstrand representation formula reads

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

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

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

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

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

The verifications of the properties of Lemmas 7.1 and 7.2 for Q_{f} and Q_{p} are done depending on [Gr, SS], but we do not present it in this article. We refer to [IS1] for the detailed presentation. In the following section we give some commutator computations that are needed in the verifications.

9 Commutator computations

The following commutators include the Mourre-type commutator, but we do not apply the Mourre theory or the limiting absorption principle [Mo, MS, GGM, FMS].

Lemma 9.1. *As a quadratic form on $C_{\mathrm{c}}^\infty(M)$, one has*

$$\begin{aligned}
\mathrm{i}[H, A] &= p_i^* (\nabla^2 r^2)^{ij} p_j + \mathrm{i}\gamma_i g^{ij} p_j - \mathrm{i} p_i^* g^{ij} \gamma_j + \gamma_0; \\
\gamma_i &= (\partial_i r^2) V + \frac{1}{4} (\partial_i \Delta r^2), \\
\gamma_0 &= (\Delta r^2) V,
\end{aligned}$$

and

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

In the application of [Gr, SS] We 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 $f'' \geq 0$. Define for any $\varepsilon \in (0,1)$ and all $t \geq 1$

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

Lemma 9.2. *There exists $\varepsilon' = \varepsilon'(\varepsilon, \kappa, \eta) > 0$ such that as a quadratic form on $C_{\mathrm{c}}^\infty(M)$*

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

These constructions are used in proving the following localization: For $e > 0$ chosen sufficiently small

$$\operatorname*{s-lim}_{t\to\infty}(I - Q_3 Q_4 Q_5^2 Q_4 Q_3)\mathrm{e}^{-\mathrm{i}tH}\chi_{[E-e,E+e]}(H) = 0; \tag{9.1}$$

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

$$-\int_1^\infty \langle \mathrm{e}^{-\mathrm{i}tH}u, (\chi^2_{-,2E_1,2E_2})'(r^2/t^2)\mathrm{e}^{-\mathrm{i}tH}u\rangle t^{-1}\,\mathrm{d}t < \infty; \tag{9.2}$$

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

$$\int_1^\infty \langle \mathrm{e}^{-\mathrm{i}tH}u, (\chi^2_{(1+\delta_3)^2E/2,(1+\delta_2)^2E/2,+})'(r^2/t^2)\mathrm{e}^{-\mathrm{i}tH}u\rangle t^{-1}\,\mathrm{d}t < \infty. \tag{9.3}$$

Given (9.1–9.3), the proofs of Lemmas 7.1 and 7.2 are very similar.

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