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Asymptotic absolute continuity for perturbed time-dependent quadratic Hamiltonians

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Abstract. We study the notion of asymptotic velocity for a class of perturbed time-dependent quadratic Hamiltonians. In particular we give a sufficient condition for absolute continuity.

Keywords. Scattering theory; quadratic Hamiltonians.

1. Introduction and results

In this paper we shall consider the question of asymptotic absolute continuity for a class of Hamiltonians $H(t) = H_0(t) + R(t, x)$ defined on $L^2(\mathbf{R}^n_x)$. The symbol of the first term, the quadratic term, is assumed to have the form

$$h_0(t; \xi, x) = \sum_{j=1}^{n} h_j(t; \xi_j, x_j);$$

$$h_j(t; \xi_j, x_j) = \frac{1}{2}\xi_j^2 + \frac{q_j}{2}x_j^2 + c_j x_j,$$

with q_j and c_j as continuous functions of a time-parameter $t > 1$. We impose a certain hyperbolicity condition which holds if for all j,

$$q_j(t) \le (2t)^{-2} \text{ for all large } t.$$

Under various conditions on the second term, the perturbation, including (as a minimum) boundedness of second order derivatives (being locally uniform in t), we study the large-time behaviour of the dynamics $U(t)$ generated by the family of $H(t)$'s.

We are interested in a generalization of the notion of *asymptotic velocity* given for $q_j = c_j = 0$ under some conditions on the potential by either of the formulas

$$f(x_t^+) = s - \lim_{t\to+\infty} U(t)^* f\left(\frac{x}{t}\right) U(t) = s - \lim_{t\to+\infty} U(t)^* f(p) U(t);$$
$$f \in C_0^\infty(\mathbf{R}^n),\ p = -i\nabla_x, \tag{1.1}$$

see ([DG], § 3.2).

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For some $\mathbf{R}^n$-valued functions L and θ given in terms of h_0 (see below), the analogous formulas are

$$f(p^+) = s - \lim_{t\to+\infty} U(t)^* f(p(t))U(t);$$

$$p_j(t) = x_j^-(t)\left(p_j - \dot{L}_j\right) + 2^{-1}\left(1 - 2\theta_j\dot{\theta}_j\right)x_j^+(t)^{-1}(x_j - L_j), \tag{1.2}$$

$$x_j^-(t) = \theta_j \mathrm{e}^{-\frac{1}{2}\int\theta_j^{-2}\mathrm{d}t}, x_j^+(t) = \theta_j \mathrm{e}^{\frac{1}{2}\int\theta_j^{-2}\mathrm{d}t}.$$

$$f(x_b^+) = s - \lim_{t\to+\infty} U(t)^* f\left(\frac{x_1 - L_1}{x_1^+(t)}, \dots, \frac{x_n - L_n}{x_n^+(t)}\right) U(t). \tag{1.3}$$

Here all arguments of f are n-tuples of commuting self-adjoint operators.

The function $x = L(t)$ is any classical solution for the symbol h_0, i.e. it solves the corresponding Newton equation. The jth entry of $\theta(t)$ is given in terms of two positive classical solutions $x_j^-(t)$ and $x_j^+(t)$ for the symbol $2^{-1}\xi_j^2 + 2^{-1}q_j x_j^2$, the former being smaller at infinity than the latter, by $\theta_j = \sqrt{x_j^+ x_j^-}$. (Notice that (1.2) and (1.3) reduce to (1.1) by the recipe $L = 0$, $x_j^- = 1$ and $x_j^+ = t$ if $q_j = c_j = 0$.)

Our first result involves an integrability condition on the first order derivatives of the symbol $r(t, x)$ of the multiplication operator $R(t, x)$.

Theorem 1.1. *Suppose that for some function $h_1 = h_1(t)$ in L^1 at infinity,*

$$|\partial_{x_j} r(t, x)| \le x_j^-(t)^{-1} h_1(t) \left(1 + \left|\left(\frac{x_1 - L_1}{x_1^+(t)}, \dots, \frac{x_n - L_n}{x_n^+(t)}\right)\right|\right). \tag{1.4}$$

Then there exist n-tuples of commuting (densely defined) self-adjoint operators, p^+ and x_b^+, given by the limits (1.2) *and* (1.3). *Moreover*

$$p^+ = x_b^+. \tag{1.5}$$

Our second result involves in addition on integrability condition on the second order derivatives of the symbol $r(t, x)$. An n-tuple of commuting self-adjoint operators is said to be absolutely continuous if its spectral measure P obeys the condition $P(\Omega) = 0$ for all Borel measurable set Ω in $\mathbf{R}^n$ with Lebesgue measure zero. If x_b^+ is absolutely continuous, the family of $H(t)$'s is said to be *asymptotic absolutely continuous.*

Theorem 1.2. *Suppose in addition to the condition* (1.4) *that for some function $h_2 = h_2(t)$ in L^1 at infinity,*

$$|\partial_{x_i}\partial_{x_j} r(t, x)| \le \min\left(x_j^+(t)^{-1}x_i^-(t)^{-1}, x_i^+(t)^{-1}x_j^-(t)^{-1}\right) h_2(t). \tag{1.6}$$

Then the family of $H(t)$'s is asymptotic absolutely continuous.

We shall prove Theorem 1.2 by showing the existence of certain wave operators. We construct unitary operators $V(t)$ with the property

$$V(t)^* p(t) V(t) = p \text{ for all large } t, \tag{1.7}$$

with $p(t)$ given in (1.2), and a smooth function $S(t, \xi)$ (smooth in ξ), such that the following result holds.

Theorem 1.3. *Under the conditions of Theorem* 1.2 *there exists the strong limit*

$$\Omega = s - \lim_{t \to +\infty} U(t)^* V(t) \mathrm{e}^{-iS(t,p)}. \tag{1.8}$$

It is a unitary operator.

Clearly Theorem 1.2 follows from Theorem 1.3 and (1.7) by the following computation

$$f(p^+) = s - \lim_{t \to +\infty} \Omega(t) f(p) \Omega(t)^* = \Omega f(p) \Omega^*;$$
$$\Omega(t) = U(t)^* V(t) \mathrm{e}^{-iS(t,p)},$$

yielding that $p^+ = \Omega p \Omega^*$.

In the case $q_j = c_j = 0$ our Theorems 1.1–1.3 essentially reduce to ([DG], Theorems 3.2.1, 3.2.2, 3.4.1), although (1.4) is weaker than ([DG], (3.4.1)) (with $|\alpha| = 1$) in that case. We have attempted to follow the procedure of [DG] as much as possible. However, since at various points the arguments of [DG] do not work in the present generality, we found it natural to give entirely self-contained proofs throughout the paper.

A main motivation for this work comes from a completeness problem in the long-range 3-body scattering theory, [Sk]. One can think about the expression $2^{-1} q_j x_j^2 + c_j x_j$ as part of a pair-potential for a system of n one-dimensional particles. We remark that while it is standard to approximate the 'inter-cluster' potential by certain time-dependent cut-offs, cf. [D, DG, E, G, H1, Si, Y1], the application of Theorem 1.2 that appears in [Sk] concerns a cut-off of the 'internal' potential as well.

The function $S(t, \xi)$ solves a certain Hamilton–Jacobi equation. The first application in scattering theory of an exact solution to a Hamilton–Jacobi equation appeared in [H1], where the existence of a certain wave operator was shown. Moreover this solution is also a powerful tool when applied to the two-body completeness problem as it was demonstrated in [Si].

Our basic strategy is to first reduce to a simpler case by replacing the symbol $2^{-1}\xi_j^2 + 2^{-1} q_j x_j^2 + c_j x_j$ by $2^{-1} a_j^2 \xi_j^2$, where $a_j = a_j(t)$ is a positive C^2-function that is not in L^2 at infinity. (In fact we shall deal with a more general unperturbed Hamiltonian than presented in this introduction. It involves a similar reduction.) The reduction is accomplished under a condition that we call as hyperbolicity condition. (Basically we need positive solutions to the unperturbed homogeneous classical equations.) We use the fact that the unperturbed dynamics is given explicitly. The closest reference we have been able to find in the literature at this point is [Y2] and the reference 4 of [Y2] (the latter in Russian), although we suspect that the explicit formula for the dynamics we are going to use (and prove) must be more widely known (at least on some form).

We shall only deal with separable unperturbed hyperbolic symbols. A natural question is whether one can generalize our results to non-separable cases. A more interesting open problem would be to understand the condition (1.6). Is it optimal for Theorem 1.2 (or 1.3) While it seems fair to say that it is 'optimal' in the case of $q_j = c_j = 0$ (see [DG], §3.8), it is not clear what to expect in the general anisotropic case.

Clearly Theorem 1.2 is a statement on propagation. A different approach to obtain related propagation estimates would be to use a certain modification of Mourre's method similar to the one used in [HS].

The above reduction is described in §§2 and 3. We give precise conditions in §4 (including one that guarantees the existence of a nice dynamics). The analogue of Theorem 1.1 is proved in §5. The function $S(t,\xi)$ is constructed in §§6 and 7 (denoted by $S_1(t,\xi)$). The analogue of Theorem 1.3 is proved in §8.

2. Hyperbolicity

We consider throughout this section quadratic symbols

$$h = h(t) = h(t;\xi,x) = \frac{a^2}{2}\xi^2 + \frac{q}{2}x^2 + cx;\, t > 1, x, \xi \in \mathbf{R}, \tag{2.1}$$

defined in terms of real-valued functions a, q and c of $t > 1$; by assumption a is C^2, and q and c are C^0. Moreover we assume $a > 0$ and that $a \notin L^2$ at infinity. By definition the *classical solutions* for $h(t)$ are the (real-valued) C^2-functions $x(t)$ which solve

$$\frac{\mathrm{d}}{\mathrm{d}t}(a^{-2}\dot{x}) = -qx - c. \tag{2.2}$$

DEFINITION 2.1

We call *h(t)* hyperbolic if there exist real-valued C^2-functions θ, y, z of large t such that $\theta, y > 0, \theta^{-2} \notin L^1$ at infinity and the corresponding classical solutions $x = x(t)$ may be written at infinity as

$$x = y(c^+ \mathrm{e}^{\int \theta^{-2}\mathrm{d}t} + c^-) + z;\, c^+, c^- \in \mathbf{R}. \tag{2.3}$$

Obviously from this definition, $h(t)$ is hyperbolic iff $h_0(t) = 2^{-1}a^2\xi^2 + 2^{-1}qx^2$ is hyperbolic. Moreover by introducing a new time variable $\tilde{t} = \int a^2\mathrm{d}t$ it follows readily that $h_0(t) = 2^{-1}a^2\xi^2 + 2^{-1}qx^2$ is hyperbolic iff $\tilde{h}_0(t) = 2^{-1}\xi^2 + 2^{-1}\tilde{q}x^2$ with $\tilde{q} = qa^{-2}$ being hyperbolic. This leads to the following criterion for hyperbolicity.

Lemma 2.2. *A symbol $h(t)$ is hyperbolic if $\tilde{q}(t) = q(t)a(t)^{-2} \leq (2t)^{-2}$ for all large t.*

Proof. We compute for $h = 2^{-1}\xi^2 + 8^{-1}t^{-2}x^2$ the solutions

$$x = t^{\frac{1}{2}}(c^+ \ln t + c^-),$$

showing that this h is hyperbolic. We construct a 'large solution' x^+ for $\tilde{h}_0(t) = 2^{-1}\xi^2 + 2^{-1}\tilde{q}x^2$ by solving the Riccati equation

$$\dot{\alpha} + \tilde{q} = -\alpha^2 \tag{2.4}$$

by comparison. The equation $\dot{\beta} + (2t)^{-2} = -\beta^2$ has the solution $\beta(t) = t^{-1}((1/2) + (1/\ln t))$. Solve (2.4) near $t = 2$ with $\alpha(2) = \beta(2)$. By the standard comparsion theorem (see for example ([BR], Theorem 1.8) we conclude that $\alpha(t) \geq \beta(t)$ for $t \geq 2$. Using (2.4) we can readily continue $\alpha(t)$ to the whole half-axis. This solution is denoted by $\alpha^+(t)$. Let $x^+ = \mathrm{e}^{\int \alpha^+ \mathrm{d}t}$. This classical solution obeys the bound $x^+(t) \geq Ct^{1/2}\ln t$, and we obtain another one, (cf. [BR], §2.5), by the formula

$$x^-(t) = x^+(t)\int_t^\infty x^+(t')^{-2}\mathrm{d}t'.$$

Let us note the following bounds

$$0 < x^-(t) = x^+(t)^{-1} \int_t^\infty \mathrm{e}^{-2\int_t^{t'} \alpha^+ \mathrm{d}t''} \mathrm{d}t'$$
$$\le x^+(t)^{-1} \int_t^\infty \left(\frac{\sqrt{t} \ln\, t}{\sqrt{t'} \ln\, t'} \right)^2 \mathrm{d}t' = x^+(t)^{-1} t\, \ln\, t \le C^{-1}\sqrt{t}.$$

Clearly (2.3) follows for $\tilde{h}_0(t)$ by writing any solution x at infinity as

$$x = x^- \left(c^+ \left(\int_t^\infty x^+(t')^{-2} \mathrm{d}t' \right)^{-1} + c^- \right); t \ge 2.$$

□

Remark 2.3.

(1) The symbol $h = 2^{-1}\xi^2 + \delta t^{-2} x^2$ is not hyperbolic for $\delta > 8^{-1}$. The classical solutions are (on complex form)

$$x = c_1 t^{2^{-1}(1+i\sqrt{8\delta-1})} + c_2 t^{2^{-1}(1+i\sqrt{8\delta-1})}.$$

There are no positive solutions at infinity.

(2) For a given hyperbolic symbol $h(t) = 2^{-1}a^2p^2 + 2^{-1}qx^2$, obviously the function θ in (2.3) obeys

$$\frac{\frac{\mathrm{d}}{\mathrm{d}t}x^+}{x^+} - \frac{\frac{\mathrm{d}}{\mathrm{d}t}x^-}{x^-} = \theta^{-2} \tag{2.5}$$

with the left hand side given in terms of the basis solutions $x^+ = y\mathrm{e}^{\int \theta^{-2}\mathrm{d}t}$ and $x^- = y$. Moreover the 'small solution' y is unique up to a constant. In terms of θ it is given by $y = a\theta \mathrm{e}^{-\frac{1}{2}\int \theta^{-2}\mathrm{d}t}$. (Notice that $a\theta = C\sqrt{x^+x^-}$.) Conversely if a symbol $h(t) = 2^{-1}a^2\xi^2 + 2^{-1}qx^2$ has positive classical solutions x^+ and x^- at infinity with the left hand side of (2.5) positive and not in L^1, then $h(t)$ is hyperbolic (just integrate (2.5)).

(3) In continuation of (2), the function θ obeys the equation

$$\ddot{\theta} + \left(a^2 q + a\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\dot{a}}{a^2} \right) \right) \theta = -\frac{1}{4}\theta^{-3}, \tag{2.6}$$

as may readily be proved from (2.5). In conjunction with (2.3) this suggests the following transformation scheme: The classical solutions x for $h(t) = 2^{-1}a^2\xi^2 + 2^{-1}qx^2$ are obtained from any solution θ to (2.6) and the classical solutions $\tilde{x}$ for $\tilde{h}(t) = 2^{-1}\tilde{a}^2\xi^2$ with $\tilde{a} = \theta^{-1}\mathrm{e}^{\frac{1}{2}\int \theta^{-2}\mathrm{d}t}$, by the transformation $x = a(\tilde{a})^{-1}\tilde{x}$. (Notice that the factor $a\tilde{(a)}^{-1}$ has the same form as the small solution mentioned in (2) confirming that the 'small $\tilde{x}$-solutions' are the constants.) A straightforward computation justifies this scheme. It is the key to handle the quantum mechanical case (see next section).

(4) Suppose we add terms $\mathrm{d}\xi x$ and $e\xi$ to the right hand side of (2.1) with d and e being C^1-functions of $t > 1$, then again the Hamilton equations reduce to (2.2) with q and c on the right hand side replaced by explicitly calculable q' and c' in C^0. Thus hyperbolicity for a general quadratic symbol reduces again to hyperbolicity for the symbol $\tilde{h}_0(t)$ used in the proof of Lemma 2.2.

3. Transformation (quantum case)

We look at the quadratic Hamiltonians given by quantizing the symbols considered in the last section:

$$H = H(t) = H(t;\, p, x) = \frac{a^2}{2}p^2 + \frac{q}{2}x^2 + cx;\, t > 1, \tag{3.1}$$

on the space $L^2(\mathbf{R}_x)$. Let $U = U(t)$ denote the corresponding evolution, fixed by $U(T) = I$ for some large $T > 1$.

We shall find U explicitly: First we reduce to the purely quadratic case in terms of any solution $x = L$ to (2.2). Let

$$\begin{aligned} U_1(t) &= \mathrm{e}^{i\int f\,\mathrm{d}t}\mathrm{e}^{-ia^{-2}\dot{L}x}\mathrm{e}^{iLp}U(t);\\ f &= \frac{q}{2}L^2 + cL - \frac{\dot{L}^2}{2a^2}. \end{aligned} \tag{3.2}$$

It solves

$$i\partial_t U_1(t) = H_1(t)U_1(t);\, H_1 = \frac{a^2}{2}p^2 + \frac{q}{2}x^2.$$

Next we pick any solution θ to (2.6) (for example the one of Definition 2.1) and introduce

$$\begin{aligned} U_2(t) &= \mathrm{e}^{igx^2}\mathrm{e}^{i\,\ln(\frac{a}{\tilde{a}})A}U_1(t); \\ g &= 4^{-1}\left(1 - 2\theta\dot{\theta} - 2\theta^2\frac{\dot{a}}{a}\right)\mathrm{e}^{-\int\theta^{-2}\mathrm{d}t},\\ \tilde{a} &= \theta^{-1}\mathrm{e}^{\frac{1}{2}\int\theta^{-2}\mathrm{d}t},\\ A &= 2^{-1}(xp + px). \end{aligned} \tag{3.3}$$

It solves

$$i\partial_t U_2(t) = H_2(t)U_2(t);\, H_2 = \frac{\tilde{a}^2}{2}p^2,$$

cf. Remark 2.3(3), and is therefore given by

$$U_2(t) = \mathrm{e}^{-i\tilde{t}\frac{p^2}{2}}U_2(T);\, \tilde{t} = \mathrm{e}^{\int_T^t\theta^{-2}\,\mathrm{d}t'}.$$

We summarize as follows:

Lemma 3.1. *For any quadratic Hamiltonian H(t) with hyperbolic symbol we let* (*for t large enough*)

$$V(t) = \mathrm{e}^{-i\int f\,\mathrm{d}t}\mathrm{e}^{-iLp}\mathrm{e}^{ia^{-2}\dot{L}x}\mathrm{e}^{-i\,\ln\left(a\theta\mathrm{e}^{-\frac{1}{2}\int\theta^{-2}\mathrm{d}t}\right)A}\mathrm{e}^{-igx^2}, \tag{3.4}$$

with L, f, g, and A given as above, *cf.* (3.2) *and* (3.3). *Then the corresponding evolution* (*for T large enough*) *is given by*

$$U(t) = V(t)\mathrm{e}^{-i\tilde{t}\frac{p^2}{2}}V(T)^{-1};\, t \geq T, \tilde{t} = \mathrm{e}^{\int_T^t\theta^{-2}\mathrm{d}t'}. \tag{3.5}$$

Motivated by Lemma 3.1 we shall call a time-dependent quadratic symbol $h(t;\xi,x)$ on $\mathbf{R}^n \times \mathbf{R}^n$ *hyperbolic* if $h(t;\xi,x) = \sum_{j=1}^n h_j(t;\xi_j,x_j)$ and each term is hyperbolic. Using Lemma 3.1 for each quantized operator $H_j(t)$ we obtain an explicit expression for the evolution $U(t)$ of the quantization $H(t)$ of $h(t;\xi,x)$. Up to the product $V(t)$ of the $V_j(t)$'s it is given as the evolution of the Hamiltonian $\tilde{H}_0(t) = \sum_{j=1}^n 2^{-1}\tilde{a}_j^2 p_j^2$.

Suppose now that we add a potential $r(t) = r(t,x)$ to a hyperbolic symbol (in $2n$-variables). Then formally (for the corresponding multiplication operator $R(t,x)$)

$$\tilde{R}(t) = \tilde{R}(t,\tilde{x}) = V(t)^{-1}R(t,x)V(t) = R(t,x(t,\tilde{x}));$$

$$x_j = a\theta_j \mathrm{e}^{-\frac{1}{2}\int \theta_j^{-2}\mathrm{d}t}\tilde{x}_j + L_j,\ j = 1,\ldots,n,$$

which leads to the study of the 'simplified' Hamiltonian $\tilde{H}(t) = \tilde{H}_0(t) + \tilde{R}(t)$.

In the next section we given precise conditions on the symbol $\tilde{r}(t,\tilde{x})$ of $\tilde{R}(t,\tilde{x})$ under which we shall study $\tilde{H}(t)$ (with the tilde-notation dropped). By the explicit nature of the transformation discussed above, they may be easily translated back to the original frame (see §1).

Remark 3.2. Suppose we add terms $d2^{-1}(px+xp)$ and ep to the right hand side of (3.1) with d and e being C^1-functions of $t > 1$, cf. Remark 2.3(4), then we may get formulas like (3.4) and (3.5). For an explicitly calculable second degree polynomial in x with time-dependent coefficients, say $h = h(t,x)$, we add the factor e^{ih} to the left on the right hand side of (3.4) and change the values of q and c according to the recipe of Remark 2.3(4) to define the other factors on the right hand side of (3.4). For the resulting $V(t) = V(t)'$, (3.5) holds. In conclusion the study of perturbations of a quadratic Hamiltonian with a more general hyperbolic symbol (of direct sum type) amounts to the study of the same 'simplified' Hamiltonian as mentioned above.

4. Conditions

We shall consider Hamiltonians $H(t)$,

$$H(t) = H_0(t) + R(t); \quad H_0(t) = \sum_{j=1}^n \frac{a_j^2}{2} p_j^2, \quad t > 1,$$

on $L^2(\mathbf{R}_x^n)$ with positive $a_j(t) \in C^0([1,\infty))$, $a_j \notin L^2$ at infinity, and with $R(t)$ given as multiplication by $r(t,x)$ obeying Conditions A, B or C given below.

We introduce the following notation:

$$b_j = b_j(t) = \int_{t_1}^t a_j^2(t')\mathrm{d}t';\ j = 1,\ldots,n, t > 1, t_1 = 1, \tag{4.1}$$

$$x_b = (x_{b1},\ldots,x_{bn});\ x_{bj} = \frac{x_j}{b_j},\ j = 1,\ldots,n,$$

$$\langle x \rangle = (1 + |x|^2)^{1/2}.$$

Condition A. The function $r(t,x) = r(t,\cdot)$ is in $C^0((1,\infty), C^2(\mathbf{R}^n))$ with $\langle x\rangle^{-2}r$, $\langle x\rangle^{-1}\partial_{x_j}r$, $\partial_{x_i}\partial_{x_j}r \in C^0((1,\infty), L^\infty(\mathbf{R}^n))$.

Condition B. In addition to Condition A, the function $r(t, \cdot)$ obeys the bounds

$$|\partial_{x_j} r| \leq h_1 \langle x_b \rangle, \tag{4.2}$$

for some $h_1 = h_1(t)$ which is in L^1 at infinity.

Condition C. In addition to Condition B, the function $r(t, \cdot)$ obeys the bounds

$$|\partial_{x_i} \partial_{x_j} r| \leq (\max(b_i, b_j))^{-1} h_2, \tag{4.3}$$

for some $h_2 = h_2(t)$ which is in L^1 at infinity.

By ([T], Theorem 7.7), Condition A is sufficient for the existence of an evolution $U(t)$ for the Hamiltonians $H(t)$ of this section. For that we notice that $S = G^2$; $G = p^2 + x^2$, is a valid input in ([T], Theorem 7.7). For each $t > 1$, $U(t)$ is a unitary operator on $L^2(\mathbf{R}^n_x)$. By ([T], (7.48) and (7.49)), $U(t)$ and $U(t)^{-1}$ preserve the domain of G, they are strongly continuous in the graph-topology on $\mathcal{D}(G)$ and the evolution has the (strong) derivative $i\partial_t U(t)\phi = H(t)U(t)\phi$ for $\phi \in \mathcal{D}(G)$. Those properties characterize $U(t)$ up to a constant factor. Notice that particular examples were given in §3.

5. Asymptotic velocity

In this section we impose Condition B. Let $U(t)$ denote the evolution fixed by $U(t) = I$ for some large T (so that $h_1 \in L^1([T, \infty])$). We shall prove the existence of an n-tuple of commuting self-adjoint operators named asymptotic velocity.

Theorem 5.1. *There exists an n-tuple of commuting self-adjoint operators* $x_b^+ = (x_{b1}^+, \ldots, x_{bn}^+)$ *on* $L^2(\mathbf{R}^n_x)$ *satisfying* (*using notation of* (4.1)) *the formulas*

$$f(x_b^+) = s - \lim_{t \to +\infty} U(t)^* f(x_b) U(t) = s - \lim_{t \to +\infty} U(t)^* f(p) U(t); \tag{5.1}$$

$$f \in C_0^\infty(\mathbf{R}^n).$$

The proof of Theorem 5.1 is given in terms of various lemmas. Let

$$X = X(t) = p^2 + (p - x_b)^2 = \sum_{j=1}^n (p_j^2 + (p_j - x_{bj})^2),$$

$$G = p^2 + x^2,$$

$$G_b = p^2 + x_b^2.$$

These operators have the common domain $\mathcal{D}(p^2) \cap \mathcal{D}(x^2)$.

Lemma 5.2. *There exists a finite constant C such that*

$$\sup_{t \geq T} ||G_b^{1/2} U(t) G^{-1/2}|| \leq C. \tag{5.2}$$

Proof. Since $U(t)$ preserves $\mathcal{D}(G)$, cf. the remark at the end of §4, it follows by interpolation that it also preserves $\mathcal{D}(G^{1/2})$. We let $\mathbf{D}$ denote the Heisenberg derivative with respect to $H(t)$ and use the notation $\langle A\rangle_t$ to denote the expectation of an observable $A = A(t)$ in a state $\phi(t) = U(t)\phi$, $\phi \in \mathcal{D}(G^{1/2})$. We compute $(\mathrm{d}/\mathrm{d}t)\langle X\rangle_t = \langle \mathbf{D}X\rangle_t$ with

$$\mathbf{D}X = -\sum_{j=1}^{n} 2\frac{a_j^2}{b_j}(p - x_b)_j^2 + Y; \tag{5.3}$$

$$Y = -p\cdot\nabla r(t,x) - \nabla r(t,x)\cdot p - (p - x_b)\cdot\nabla r(t,x) - \nabla r(t,x)\cdot(p - x_b).$$

Since

$$Y \leq \sqrt{n}h_1(2 + 5X), \tag{5.4}$$

we get by invoking the Gronwall inequality

$$\langle X(t)\rangle_t \leq C_1(\langle X(T)\rangle_T + ||\phi||^2) \leq C_2||G^{1/2}\phi||^2.$$

□

Lemma 5.3. *There exists an n-tuple of commuting self-adjoint operators* p^+ *on* $L^2(\mathbf{R}_x^n)$ *satisfying the following formula for all* $f \in C_0^\infty(\mathbf{R}^n)$,

$$f(p^+) = s - \lim_{t\to+\infty} U(t)^* f(p)U(t). \tag{5.5}$$

Proof. We compute for $\phi, \psi \in \mathcal{D}(G^{1/2})$, $(\mathrm{d}/\mathrm{d}t)\langle\psi(t), f(p)\phi(t)\rangle = \langle\psi(t), \mathbf{D}f(p)\phi(t)\rangle$ with

$$\mathbf{D}f(p) = -i(2\pi)^{-n/2}\int_{\mathbf{R}^n}\hat{f}(y)\int_0^1 \mathrm{e}^{i(1-\sigma)p\cdot y}y\cdot\nabla r(t,x)\mathrm{e}^{i\sigma p\cdot y}\mathrm{d}\sigma\mathrm{d}y, \tag{5.6}$$

given in terms of the Fourier transform of f.

Using the bounds (4.2),

$$||\langle x_b\rangle \mathrm{e}^{i\sigma p\cdot y}\langle x_b\rangle^{-1}|| = ||\langle x_b - \sigma y_b\rangle x_b\rangle^{-1}|| \leq \sqrt{2}\langle y_b\rangle$$

and (5.2), we get from (5.6) that

$$||\mathbf{D}f(p)\phi(t)|| \leq C_1h_1||G_b^{1/2}\phi(t)|| \leq C_2||G^{1/2}\phi||h_1 = C_3h_1.$$

Consequently (by integrating) there exists the limit on the right hand side of (5.5).

The fact that p^+ is densely defined follows from the bound

$$||1_{\{|p|\geq\kappa\}}\phi(t)|| \leq \kappa^{-1}|||p|\phi(t)|| \leq \kappa^{-1}C||G^{1/2}\phi||,$$

valid for all $\kappa > 0$ with C given by (5.2). □

Lemma 5.4. *There exists a finite constant C such that for all* $\phi(t) = U(t)\phi$, $\phi \in \mathcal{D}(G^{1/2})$, *and* $j = 1, \ldots, n$

$$\int_T^\infty ||(p_j - x_{b_j})\phi(t)||^2\frac{a_j^2}{b_j}\,\mathrm{d}t \leq C||G^{1/2}\phi||^2. \tag{5.7}$$

Proof. We use (5.3), (5.4) and (5.2) to estimate

$$\int_T^\infty ||(p_j - x_{b_j})\phi(t)||^2 \frac{a_j^2}{b_j} \mathrm{d}t \le \langle X(T)\rangle_T + \int_T^\infty \sqrt{n} h_1 \langle 2 + 5X\rangle_s \mathrm{d}s \le C||G^{1/2}\phi||^2.$$

□

We notice that the factors $a_j^2 b_j^{-1}$ in (5.7) do not belong to L^1. Consequently along a sequence $t = t_m \to +\infty$ (possibly depending on ϕ and j),

$$||(p_j - x_{bj})\phi(t_m)|| \to 0. \tag{5.8}$$

Lemma 5.5. *With* $\phi(t) = U(t)\phi$, $\phi \in \mathcal{D}(G^{1/2})$,

$$|||(p - x_b)|\phi(t)|| \to 0 \quad \textit{for} \quad t \to +\infty. \tag{5.9}$$

Proof. Let $\Phi_j(t) = (p_j - x_{b_j})^2$. We compute, cf. (5.3),

$$\langle \mathbf{D}\Phi_j\rangle_t = \left\langle -2\frac{a_j^2}{b_j}(p - x_b)_j^2 \right\rangle_t - \langle (p - x_b)_j(\partial_{x_j} r)(t, x) + (\partial_{x_j} r)(t, x)(p - x_b)_j\rangle_t.$$

By (5.7) the first term on the right hand side is in L^1. As for the second term $|\langle\cdot\rangle_t| \le h_1\langle 1 + 3X\rangle_t$, cf. (5.4). Consequently by Lemma 5.2 also this term is in L^1. We conclude that $\langle\Phi_j\rangle_t \to C_j$, whence by (5.8), $C_j = 0$. □

Lemma 5.6. *With* p^+ *given as in Lemma* 5.3, *for all* $f \in C_0^\infty(\mathbf{R}^n)$,

$$s - \lim_{t\to+\infty} U(t)^* f(x_b) U(t) = f(p^+). \tag{5.10}$$

Proof. By the Baker–Campbell–Hausdorff formula (cf. [DG], (3.2.28)) (or by other means)

$$f(p) - f(x_b) = B_1(p - x_b) + B_2$$

with $||B_1|| = O(t^0)$ and $||B_2|| = O(\max(b_1^{-1}, \dots, b_n^{-1})) = o(t^0)$. Applied to $\phi(t) = U(t)\phi$ with $\phi \in \mathcal{D}(G^{1/2})$, we get the conclusion from (5.9). □

6. A fixed point problem

In this and the next sections we impose Condition C. Here we shall study an inversion problem for the classical solutions for the symbol

$$h = h(t; \xi, x) = \sum_{j=1}^n 2^{-1} a_j(t)^2 \xi_j^2 + r(t, x). \tag{6.1}$$

We shall follow the procedure of ([DG], §1.5). Consider for fixed (large) $T > 1$, and given $t \in [T, \infty)$ and $\xi \in \mathbf{R}^n$, the classical solution which at time $s = T$ has position 0 and at time $s = t$ has momentum ξ:

$$\begin{aligned} \partial_s y_j(s,t,\xi) &= a_j^2(s)\eta_j(s,t,\xi), \\ \partial_s \eta_j(s,t,\xi) &= -(\partial_{x_j} r)(s, y(s,t,\xi)), \\ y_j(T,t,\xi) &= 0, \\ \eta_j(t,t,\xi) &= \xi_j;\ j = 1,\dots,n. \end{aligned} \tag{6.2}$$

We shall show that (6.2) has a unique solution (y, η).

For a solution $(y(s), \eta(s))$ we introduce with b_j given as in (4.1) but now with $t_1 = T$ (explicity $b_j(s) = \int_T^s a_j^2(t')\mathrm{d}t'$),

$$z_j(s) = y_j(s) - b_j(s)\xi_j;\ j = 1,\dots,n. \tag{6.3}$$

Then, putting $b(u) = (b_1(u), \dots, b_n(u))$, $z = (z_1, \dots, z_n)$ solves the integral equations

$$\begin{aligned} z_j(s) &= \int_T^t \zeta_{s,j}(u)(\partial_{x_j} r)(u, z(u) + b(u)\cdot\xi)\mathrm{d}u; \\ \zeta_{s,j}(u) &= \begin{cases} b_j(u), & u \le s \\ b_j(s), & s < u \end{cases},\ s, u \ge T,\ j = 1,\dots,n. \end{aligned} \tag{6.4}$$

Conversely a solution z to (6.4) defines a solution (y, η) to (6.2) by the formula (6.3). We shall show that (6.4) has a unique solution. For that it is convenient to introduce the notation

$$z_b = z_b(s) = z_{b(s)}(s) = \left(b_1(s)^{-1}z_1(s), \dots, b_n(s)^{-1}z_n(s)\right), \tag{6.5}$$

and to consider the space

$$Z_t = \left\{ z \in C^0([T,t], \mathbf{R}^n) \mid ||z|| := \sup_{T \le s \le t} |z_b(s)| < \infty \right\}. \tag{6.6}$$

Obviously any solution z to (6.4) belongs to Z_t.

We define for $z \in Z_t$, $\mathcal{P}(z)$ to be the $\mathbb{R}^n$-valued function whose jth coordinate is the expression on the right hand side of (6.4). We claim that $\mathcal{P}$ is a contraction on Z_t. Using the bound

$$b_j(s)^{-1}\zeta_{s,j}(u) \le 1, \tag{6.7}$$

it follows from (4.2) that for all $z \in Z_t$,

$$\begin{aligned} b_j(s)^{-1}|(\mathcal{P}(z))_j(s)| &\le \int_T^t h_1(u)\left(1 + |z_{b(u)}(u)| + |\xi|\right)\mathrm{d}u \\ &\le (1 + ||z|| + |\xi|)||h_1||_{L_T^1};\ L_T^1 = L^1([T,\infty)), \end{aligned} \tag{6.8}$$

showing that $\mathcal{P}$ maps into Z_t.

Next, from (4.3) we get the bound

$$|(\partial_{x_j} r)(u, z_1(u) + b(u)\cdot\xi) - (\partial_{x_j} r)(u, z_2(u) + b(u)\cdot\xi)|$$
$$\leq \sqrt{n} h_2(u)|z_{1,b(u)}(u) - z_{2,b(u)}(u)|,$$

showing together with (6.7) that for T large enough

$$||\mathcal{P}(z_1) - \mathcal{P}(z_2)|| \leq n||h_2||_{L^1_T}||z_1 - z_2|| \leq 2^{-1}||z_1 - z_2||. \tag{6.9}$$

It follows that indeed $\mathcal{P}$ is a contraction. Whence by the fixed point theorem $z = \mathcal{P}(z)$ has a unique solution in Z_t.

We have the following properties:

Lemma 6.1. *The unique solution* (y, η) *to* (6.2) *obeys the following bounds as* $t \to \infty$ *which are uniform in* $\xi \in \mathbf{R}^n$,

$$\partial_\xi^\beta (y_j(t) - b_j(t)\xi_j) = o(t^0) b_j(t)\langle\xi\rangle^{1-|\beta|};$$
$$|\beta| \leq 1,\ j = 1, \dots, n. \tag{6.10}$$

Proof. If $\beta = 0$, we show the bounds (6.10) as follows: By estimating and subtracting in (6.8),

$$\left(1 - \sqrt{n}||h_1||_{L^1_T}\right)||z|| \leq \sqrt{n}(1 + |\xi|)||h_1||_{L^1_T}. \tag{6.11}$$

Assuming that $\sqrt{n}||h_1||_{L^1_T} \leq 2^{-1}$, (6.11) yields

$$||z|| \leq (1 + |\xi|). \tag{6.12}$$

Next by keeping the factor $b_j(s)^{-1}\zeta_{s,j}(u)$ in the estimates (6.8) and using (6.12) we get the bound

$$|z_b(s)| \leq 2\sqrt{n}(1 + |\xi|)\int_T^\infty f_s(u) h_1(u)\mathrm{d}u;$$
$$f_s(u) = \sup_{j=1,\dots,n} b_j(s)^{-1}\zeta_{s,j}(u) (\leq 1). \tag{6.13}$$

Since for fixed $u \in [T, \infty)$, $\lim_{s\to\infty} f_s(u) = 0$, we conclude from (6.13) (with $s = t$) by using the Lebesgue dominated convergence theorem that indeed the bounds (6.10) hold for $\beta = 0$.

To handle the case $|\beta| = 1$ we notice that for all $i = 1, \dots, n$ and $z \in Z_t$,

$$((\partial_{\xi_i}\mathcal{P})(z))_j(s) = \int_T^t \zeta_{s,j}(u) b_i(u)(\partial_{x_i}\partial_{x_j} r)(u, z(u) + b(u)\cdot\xi)\mathrm{d}u, \tag{6.14}$$

and therefore, cf. (6.9) and (6.13), that $\left(\partial_{\xi_i}\mathcal{P}\right)(z) \in Z_t$ with

$$||(\partial_{\xi_i}\mathcal{P})(z)|| \leq 2^{-1}, \tag{6.15}$$

and

$$|((\partial_{\xi_i}\mathcal{P})(z))_b(t)| \leq \sqrt{n}\int_T^\infty f_t(u) h_2(u)\mathrm{d}u. \tag{6.16}$$

Similarly

$$((\nabla_z \mathcal{P})(z)\tilde{z})_j(s) = \sum_{i=1}^{n} \int_T^t \zeta_{s,j}(u)(\partial_{x_i}\partial_{x_j} r)(u, z(u) + b(u) \cdot \xi)\tilde{z}_i(u)\mathrm{d}u, \tag{6.17}$$

yielding that $\mathcal{P}$ is differentiable on Z_t with

$$||(\nabla_z \mathcal{P})(z)|| \leq 2^{-1}, \tag{6.18}$$

and

$$|((\nabla_z \mathcal{P})(z)\tilde{z})_b(t)| \leq n||\tilde{z}||_{Z_t} \int_T^\infty f_t(u)h_2(u)\mathrm{d}u. \tag{6.19}$$

By differentiating $z = \mathcal{P}(z)$ we get (at least formally)

$$\partial_{\xi_i} z = (\partial_{\xi_i} \mathcal{P})(z) + (\nabla_z \mathcal{P})(z)\partial_{\xi_i} z, \tag{6.20}$$

which when combined with (6.15) and (6.18) gives that $\partial_{\xi_i} z \in Z_t$ with

$$||\partial_{\xi_i} z|| \leq 1. \tag{6.21}$$

By using (6.16), (6.19) and (6.21) to the right hand side of (6.20) we finally conclude (invoking again the Lebesgue dominated convergence theorem) that

$$(\partial_{\xi_i} z)_b(t) = o(t^0) \text{ uniformly in } \xi. \tag{6.22}$$

□

Remark 6.2.

(1) By using similar arguments as those appearing in the last part of the proof of Lemma 6.1 one readily obtains that $\partial_t z \in Z_t$.
(2) If r is C^k in x for $k \geq 3$ with locally bounded higher order derivatives one obtains by differentiating (6.20) that z is C^{k-1} in ξ with locally bounded higher order derivatives.
(3) One may choose $t = \infty$ in (6.4). Similarly estimating one shows that $\partial_\xi^\beta z \in Z_\infty$ for $|\beta| = 1$. An easy application of this estimate yields that for all large enough s, the map $\mathbf{R}^n \ni \xi \to \eta(s, \infty, \xi) \in \mathbf{R}^n$ is bijective.

7. Construction of phase functions

We shall solve a Hamilton–Jacobi equation in terms of the solution (y, η) to (6.2). We use the procedure of ([DG], Theorem A.3.1).

Let for $t \geq T$ and $\xi \in \mathbf{R}^n$,

$$S(t, \xi) = \int_T^t (h(u; \eta(u), y(u)) + y(u) \cdot \partial_u \eta(u))\mathrm{d}u, \tag{7.1}$$

with h given by (6.1) and

$$y(s) = y(s, t, \xi) \quad \text{and} \quad \eta(s) = \eta(s, t, \xi).$$

Then by straightforward calculations using Lemma 6.1 and Remark 6.2(1) we get

$$\begin{aligned} \partial_t S(t,\xi) &= h(t;\xi,\nabla_\xi S(t,\xi)),\\ S(T,\xi) &= 0,\\ y(t,t,\xi) &= \nabla_\xi S(t,\xi). \end{aligned} \tag{7.2}$$

Obviously by combining Lemma 6.1 and (7.2) we get estimates of the first and second order ξ-derivatives of $S(t,\xi)$.

For technical reasons we shall need the existence of higher order derivatives (and bounds of those). For that we need higher order derivatives of r, cf. Remark 6.2(2). More precisely we shall decompose r into a sum of a short-range term and a smooth term, cf. ([DG], Lemma 3.4.5(ii)), and then define S by the above formula in terms of the latter input.

Pick $j \in C_0^\infty(\mathbf{R}^n)$ with $\int j(x)\mathrm{d}x = 1$ and $\int xj(x)\mathrm{d}x = 0$. We decompose $r = r_s + r_1$ with

$$r_1 = \int r\left(t, x + b^{1/2}(t)\cdot y\right) j(y)\mathrm{d}y; \quad b^{1/2} = \left(b_1^{1/2}, \dots, b_n^{1/2}\right). \tag{7.3}$$

By Taylor expansion one obtains a bound of r_s in terms of the expressions $b_i^{1/2}(t)b_j^{1/2}(t)||\partial_i\partial_j r(t,\cdot)||_\infty$, which by Condition C are in L^1. So

$$||r_s(t,\cdot)||_\infty \in L^1. \tag{7.4}$$

As for r_1 we have the uniform estimates

$$|\partial_x^{\alpha+e_i+e_j} r_1| \le (\max(b_i,b_j))^{-1} b^{-\alpha/2} h, \tag{7.5}$$

valid for all multi-indices α and $i, j = 1, \dots, n$. Here e_i denotes the ith standard vector in $\mathbf{R}^n$, $b^v = \Pi_{l=1}^n b_l^{v_l}$ (for $v \in \mathbf{R}^n$), and $h = h_\beta \in L^1(\mathrm{d}t)$. In particular r_1 obeys Condition C.

Next we define S_1 by (7.1) with the input r_1. We prove the following analogue of ([DG], Proposition 3.4.3) (by a different proof).

Lemma 7.1. *For all multi-indices β, $1 \le i, j \le n$ and all large t,*

$$|\partial_\xi^{\beta+e_i+e_j} S_1| \le C_\beta \min(b_i, b_j) b^{\beta/2}. \tag{7.6}$$

Proof. First we notice that S_1 is indeed smooth in ξ with locally bounded derivatives (of order ≥ 2), cf. Remark 6.2(2).

We proceed by induction in $|\beta|$. For $|\beta| = 0$, (7.6) follows from Lemma 6.1.

Suppose (7.6) for $|\beta| \le k-1$; $k \ge 1$. Then we need to bound the derivatives of order $|\beta| = k$.

We introduce the shorthand notation

$$f_{\gamma,i,j} = \partial_\xi^{\gamma+e_i+e_j} S_1(t,\xi),\ g_{\gamma,i,j} = b^{-\frac{\gamma}{2}-e_i}|f_{\gamma,i,j}|,\ f_\gamma = \partial_\xi^\gamma S_1(t,\xi).$$

Let

$$X = \sum_{|\gamma|=k; i,j\le n} g_{\gamma,i,j}^2.$$

It suffices to show that for some $T' > T$

$$\sup_{t \geq T', \xi \in \mathbf{R}^n} |X(t, \xi)| < \infty. \tag{7.7}$$

For that we shall prove a differential inequality. The derivative of $f_{\gamma,i,j}$ is computed by differentiating the Hamilton–Jacobi equation in (7.2):

$$\frac{\mathrm{d}}{\mathrm{d}t} f_{\gamma,i,j} - \nabla r_1 \cdot \nabla f_{\gamma,i,j} = \sum_{\substack{k+2 \geq l \geq 2 \\ \sum \gamma_l = \gamma + e_i + e_j}} C_{l,\gamma_1,\ldots,\gamma_l} \left(\nabla^l r_1\right) (\nabla f_{\gamma_1}, \ldots, \nabla f_{\gamma_l}).$$

On the right hand side some terms can be estimated by the induction hypothesis; the others in terms of some $f_{\gamma',i',j'}$ with $|\gamma'| = k$. In both cases there are two sub-cases depending on whether the ith and the jth derivatives 'hit' the same factor of ∇S_1 or two different ones. There are terms, all subject to the condition $\gamma_1 + \cdots + \gamma_l = \gamma$,

$$(\partial_{q_1} f_{\gamma_1,i,j})(\partial_{q_2} f_{\gamma_2}) \partial_{q_1} \partial_{q_2} r_1;\ |\gamma_1| = k - 1, \tag{7.8}$$

$$(\partial_{q_1} f_{\gamma_1+e_i})(\partial_{q_2} f_{\gamma_2+e_j}) \partial_{q_1} \partial_{q_2} r_1;\ \gamma_1 = 0 \text{ or } \gamma_2 = 0, \tag{7.9}$$

$$(\partial_{q_1} f_{\gamma_1,i,j})(\partial_{q_2} f_{\gamma_2})(\nabla^{l-2} \partial_{q_1} \partial_{q_2} r_1)(\nabla f_{\gamma_3}, \ldots, \nabla f_{\gamma_l});\ |\gamma_1| \leq k - 2, \tag{7.10}$$

$$(\partial_{q_1} f_{\gamma_1+e_i})(\partial_{q_2} f_{\gamma_2+e_j})(\nabla^{l-2} \partial_{q_1} \partial_{q_2} r_1)(\nabla f_{\gamma_3}, \ldots, \nabla f_{\gamma_l});\ |\gamma_1|, |\gamma_2| \leq k - 1. \tag{7.11}$$

As for the terms of the form (7.8) we estimate the first factor

$$|\partial_{q_1} f_{\gamma_1,i,j}| \leq C g_{\gamma_1+e_{q_1},i,j} b^{\frac{\gamma_1+e_{q_1}}{2}} b_i,$$

the second factor

$$|\partial_{q_2} f_{\gamma_2}| \leq C b_{q_2}^{1/2} b^{\frac{\gamma_2}{2}},$$

and the last factor

$$|\partial_{q_1} \partial_{q_2} r| \leq b_{q_1}^{-\frac{1}{2}} b_{q_2}^{-\frac{1}{2}} h_2,$$

yielding altogether the upper bound

$$C b_i b^{\gamma/2} g_{\gamma_1+e_{q_1},i,j} h_2.$$

As for the terms of the form (7.9) we estimate in the case $\gamma_2 = 0$, the first factor

$$|\partial_{q_1} f_{\gamma_1+e_i}| \leq C g_{\gamma,i,q_1} b^{\gamma/2} b_i,$$

the second factor

$$|\partial_{q_2} f_{e_j}| \leq b_{q_2},$$

and the last factor

$$|\partial_{q_1} \partial_{q_2} r_1| \leq b_{q_2}^{-1} h_2,$$

yielding the upper bound

$$Cb_i b^{\gamma/2} g_{\gamma,i,q_1} h_2.$$

Similarly if $\gamma_1 = 0$ in (7.9) we get the upper bound

$$Cb_i b^{\gamma/2} g_{\gamma,q_2,j} h_2.$$

As for the terms of the form (7.10) or (7.11) we proceed similarly noticing that all appearing f's are of lower order, which means that they can be estimated by the induction hypothesis. The factors to the right (for $l \geq 3$) are estimated as

$$|f_{\gamma_m + e_{q_m}}| \leq Cb^{(\gamma_m + e_{q_m})/2}.$$

In conclusion these terms have the upper bound

$$b_i b^{\gamma/2} h$$

with h in L^1.

We finally conclude that for some h in L^1,

$$\left| \frac{\mathrm{d}}{\mathrm{d}t} f_{\gamma,i,j} - \nabla r_1 \cdot \nabla f_{\gamma,i,j} \right| \leq b_i b^{\gamma/2} h \left(1 + \sum_{|\gamma'|=k} g_{\gamma',i',j'} \right). \tag{7.12}$$

But if $\xi(t)$ solves

$$\frac{\mathrm{d}}{\mathrm{d}t} \xi = -\nabla_x r_1(t, \nabla_\xi S_1(t, \xi)),$$

then

$$\frac{\mathrm{d}}{\mathrm{d}t} f_{\gamma,i,j} - \nabla r_1 \cdot \nabla f_{\gamma,i,j} = \frac{\mathrm{d}}{\mathrm{d}t} f_{\gamma,i,j}(t, \xi(t)).$$

Since the coordinates of b are increasing, (7.12) consequently leads to

$$\frac{\mathrm{d}}{\mathrm{d}t} X = \frac{\mathrm{d}}{\mathrm{d}t} X(t, \xi(t)) \leq h(X + 1),$$

and therefore by the Gronwall inequality to

$$X(t, \xi(t)) \leq C_1(X(T', \xi(T')) + 1) \leq C_2; t \geq T' = T + 1, \tag{7.13}$$

cf. Remark 6.2(2).

We apply (7.13) to $\xi(t)$ defined by $\xi(t) = \eta(t, \infty, \xi')$, cf. Remark 6.2(3). By this remark, the map $\xi' \to \eta(t, \infty, \xi')$ is onto for all large enough t, which shows (7.7). □

8. Wave operators

Under Condition C and with $S_1(t, \eta)$, the function constructed in §7 we introduce the Møller wave operators

$$W = s - \lim_{t \to +\infty} \mathrm{e}^{iS_1(t,p)} U(t), \Omega = s - \lim_{t \to +\infty} U(t)^* \mathrm{e}^{-iS_1(t,p)}. \tag{8.1}$$

(Here p is the momentum operator $p = -i\nabla$.) Our main result is the following.

Theorem 8.1. *There exist the strong limits in* (8.1).

For convenience we shall only prove the existence of W. (The existence of Ω is easier to prove.) We shall use the chain rule for wave operators. Obviously by (7.4) we may replace r by r_1 (and logically replace $U(t)$ by $U_1(t)$). For convenience we drop from this point the subindex '1' and thus aim at showing the existence of

$$\lim_{t\to+\infty} \mathrm{e}^{iS(t,p)}U(t)\phi;\ \phi\in L^2(\mathbf{R}^n).$$

By Lemma 5.2 we may insert a factor $F(X)$ where $F\in C^\infty(\mathbf{R})$ with $F'\leq 0$, $F(s)=1$ for $s\leq C$, $F(s)=0$ for $s\geq 2C$, and with $X=X(t)$ given as in §5. (We just need to pick $C>0$ large enough.) So it suffices to prove the existence of

$$\lim_{t\to+\infty} \mathrm{e}^{iS(t,p)}F(X)U(t)\phi.$$

We need an analogue of ([DG], Lemma 3.4.7). It involves a generalized Baker–Campbell–Hausdorff formula.

Lemma 8.2. *We can write*

$$R(t,x)-R(t,\nabla_\xi S(t,p)) = A(t)\cdot(x-\nabla_\xi S(t,p))+B(t); \tag{8.2}$$
$$A(t)=\int_0^1(\nabla_x r)(t,\nabla_\xi S(t,p)+\sigma(x-\nabla_\xi S(t,p)))\mathrm{d}\sigma,$$
$$||B(t)||\in L^1.$$

Proof. We represent the left hand side of (8.2) as

$$\int_0^1 \frac{\mathrm{d}}{\mathrm{d}\sigma}\left(\mathrm{e}^{i((1-\sigma)/\sigma)S}R(t,\sigma x)\mathrm{e}^{-i((1-\sigma)/\sigma)S}\right)\mathrm{d}\sigma,$$

and compute the derivative of each of the three factors. This yields the representation

$$B(t)=\int_0^1 \mathrm{e}^{i((1-\sigma)/\sigma)S}B(t,\sigma)\mathrm{e}^{-i((1-\sigma)/\sigma)S}\mathrm{d}\sigma;$$
$$B(t,\sigma)=-i\sigma^{-2}[S(t,p),R(t,\sigma x)]+\sigma^{-1}(\nabla r)(t,\sigma x)\cdot(\nabla S)(t,p).$$

The operator $B(t,\sigma)$ has the symbol

$$b_{t,\sigma}(x,y,\xi)$$
$$=\sum_{|\beta|=2}\frac{2}{\beta!}i(2\pi)^{-n}\int_0^1(1-s)\mathrm{e}^{i(x-y)\cdot\xi}\left(\partial_x^\beta r\right)(t,\sigma(x+s(y-x)))\partial_\xi^\beta S(t,\xi)\mathrm{d}s.$$

By (7.5) and (7.6), for all multi-indices α_1,α_2 and β,

$$|\partial_x^{\alpha_1}\partial_x^{\alpha_2}\partial_\xi^\beta b_{t,\sigma}|\leq b^{(\alpha_1+\alpha_2)/2}b^{-\beta/2}h, \tag{8.3}$$

with h in $L^1(\mathrm{d}t)$ and depending only on the multi-indices.

Using a scaling and the Calderón–Vaillancourt theorem (cf. ([DG], Proposition D.5.1), [CV] or ([H2], Theorem 18.6.3)), it follows from (8.3) that indeed

$$\sup_{\sigma\in[0,1]}||B(\cdot,\sigma)||\in L^1.$$

□

Next following ([DG], §3.4) we introduce $\tilde{H}(t) = H(t) - B(t)$ with $B(t)$ given by (8.2). Using again ([T], Theorem 7.7) we conclude that $\tilde{H}(t)$ generates a propagator, denoted as $\tilde{U}(t)$, which preserves the domain of $G = p^2 + x^2$. Obviously by Lemma 8.2,

$$\sup_t ||\tilde{U}(t)|| < \infty. \tag{8.4}$$

Lemma 8.3. *There exists*

$$s - \lim_{t\to+\infty} \tilde{U}(t)^* F(X) U(t). \tag{8.5}$$

Proof. Using Lemma 8.2 and (8.4) it suffices to verify (suitably) integrability of $\tilde{U}(t)^* \mathbf{D} F(X) U(t)\phi$ with $\mathbf{D}$ given as in the proof of Lemma 5.2.

We compute in terms of an almost analytic extension $\tilde{F}$,

$$\mathbf{D}F(X) = -\frac{1}{\pi}\int_{\mathbf{C}} \left(\bar{\partial}\tilde{F}\right)(w)(X-w)^{-1}\mathbf{D}X(X-w)^{-1}\mathrm{d}u\mathrm{d}v. \tag{8.6}$$

Here $\mathbf{D}X$ is given by (5.3). The contribution from the second term Y on the right hand side of (5.3) is integrable. The contribution from the first term is the non-negative operator

$$-\sum_{j=1}^n 2\frac{a_j^2}{b_j}(p-x_b)_j F'(X)(p-x_b)_j = \sum_{j=1}^n B_j^* B_j;$$

$$B_j = \left(-2\frac{a_j^2}{b_j}F'(X)\right)^{1/2}(p-x_b)_j.$$

We need the estimates

$$\int_T^\infty ||B_j U(t)\phi||^2 \mathrm{d}t \le C||\phi||^2, \tag{8.7}$$

$$\int_T^\infty ||B_j \tilde{U}(t)\psi||^2 \mathrm{d}t \le C||\psi||^2. \tag{8.8}$$

These estimates follow by differentiating the uniformly bounded families $U(t)^* F(X) U(t)$ and $\tilde{U}(t)^* F(X)\tilde{U}(t)$, respectively, under use of the above computation.

We conclude from (8.7) and (8.8) that indeed

$$\lim_{t_1\to+\infty}\sup_{t_2\ge t_1}\left|\left|\int_{t_1}^{t_2}\tilde{U}(t)^* B_j^* B_j U(t)\phi\mathrm{d}t\right|\right| = 0,$$

completing the proof. □

Due to Lemma 8.3 it remains to prove the existence of

$$\lim_{t\to+\infty} \mathrm{e}^{iS(t,p)} F(X)\check{\phi}(t);\ \check{\phi}(t) = \tilde{U}(t) G^{-1/2}\phi,\ G = p^2 + x^2.$$

For that we proceed by differentiating as in the proof of Lemma 8.3. We notice the bound

$$\int_T^\infty ||B_j \mathrm{e}^{-iS(t,p)}\psi||^2 \mathrm{d}t \le C||\psi||^2, \tag{8.9}$$

which follows by the same method as the one used to prove (8.7) and (8.8) (and under use of Lemma 6.1). Using (8.8) and (8.9) it suffices to show integrability of

$$i[r(t, \nabla_\xi S(t,p)), F(X)]\check{\phi}(t), \tag{8.10}$$

and

$$F(X)A(t)\cdot(x - \nabla_\xi S(t,p))\check{\phi}(t). \tag{8.11}$$

As for (8.10) we have a similar representation of the commutator as given in (8.6) and we invoke Lemma 6.1 again.

As for (8.11) we notice that

$$||F(X)A(t)|| \in L^1(\mathrm{d}t), \tag{8.12}$$

(since this bound holds for $X^{-1/2}A(t)$).

The function

$$f(t) = ||(x - \nabla_\xi S(t,p))\check{\phi}(t)||^2$$

obeys, cf. the proof of ([DG], Lemma 3.4.9) (or [Si]),

$$\frac{\mathrm{d}}{\mathrm{d}t} f(t) = \sum_{k,l\le n} \Big\langle (x_k - \partial_{\xi_k} S(t,p))\check{\phi}(t), A_{kl}(x_l - \partial_{\xi_l} S(t,p))\check{\phi}(t)\Big\rangle + \text{h.c.};$$

$$A_{kl} = i[A_l, (x_k - \partial_{\xi_k} S(t,p))],\ A(t) = (A_1, \dots, A_n).$$

We compute

$$A_{kl} = \int_0^1 \mathrm{e}^{i((1-\sigma)/\sigma)S} A_{kl}(t,\sigma)\mathrm{e}^{-i((1-\sigma)/\sigma)S}\mathrm{d}\sigma;$$
$$A_{kl}(t,\sigma) = i\sigma^{-1}[\partial_{\xi_k} S(t,p), (\partial_{x_l} r)(t,\sigma x)].$$

The operator $A_{kl}(t,\sigma)$ has the symbol

$$a_{kl}(t,\sigma; x, y, \xi) = \sum_{j=1}^n (2\pi)^{-n} \int_0^1 \mathrm{e}^{i(x-y)\cdot\xi} (\partial_{x_j}\partial_{x_l} r)(t, \sigma(x + s(y-x)))\partial_{\xi_j}\partial_{\xi_k} S(t,\xi)\mathrm{d}s.$$

It obeys the same estimates as $b_{t,\sigma}$ in (8.3), and consequently $||A_{kl}|| \in L^1$.

We conclude that

$$\frac{\mathrm{d}}{\mathrm{d}t} f(t) \le h(t)f(t)$$

with $h \in L^1$, whence it follows by the Gronwall inequality that

$$f(t) \le C;\ t \ge T'. \tag{8.13}$$

By combining (8.12) and (8.13) we finally conclude that indeed the expression (8.11) is integrable. The proof of the existence of the wave operator W is complete.

References

[BR] Birkhoff G and Rota G C, Ordinary differential equations, 4th edition (New York: John Wiley & Sons) (1989)

[CV] Calderón A P and Vaillancourt R, On the boundedness of pseudo-differential operators, *J. Math. Soc. Jpn.* **23(2)** (1971) 374–378

[D] Dereziński J, Asymptotic completeness for N-particle long-range quantum systems, *Ann. Math.* **138** (1993) 427–476

[DG] Dereziński J and Gérard C, Scattering theory of classical and quantum N-particle systems, *Texts Monogr. Phys.* (Berlin, Heidelberg, New York: Springer) (1997)

[E] Enss V, Long-range scattering of two- and three-body quantum systems, Journées Equations à Dérivées Partielles, Saint Jean de Monts, Juin, 1989, Publ. Ecole Polytechnique, Palaiseau (1989) pp. 1–31

[G] Gérard C, Asymptotic completeness for 3-particles systems, *Invent. Math.* **114** (1993) 333–397

[HS] Herbst I and Skibsted E, Quantum scattering for homogeneous of degree zero potentials: Absence of channels at local maxima and saddle points (MaPhySto) (1999) preprint 24

[H1] Hörmander L, The existence of wave operators in scattering theory, *Math. Z.* **146** (1976) 69–91

[H2] Hörmander L, The analysis of linear partial differential operators III (Berlin: Springer-Verlag) (1985)

[Si] Sigal I M, On the long range scattering, *Duke. Math. J.* **60** (1990) 473–492

[Sk] Skibsted E, Long-range scattering of three-body quantum systems II, submitted

[T] Tanabe H, Functional analytic methods for partial differential equations (New York: Marcel Dekker) (1997)

[Y1] Yafaev D, New channels of scattering for three-body quantum systems with long-range potentials, *Duke Math. J.* **82(3)** (1996) 553–584

[Y2] Yafaev D, On the asymptotic behavior of solutions of the time-dependent Schrödinger equation, *Math. USSR Sbornik* **39(2)** (1981) 169–188