TIME–DEPENDENT SCATTERING THEORY OF N–BODY QUANTUM SYSTEMS

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Abstract. We give a full and selfcontained account of the basic results in N–body scattering theory which emerged over the last ten years: The existence and completeness of scattering states for potentials decreasing like $r^{-\mu}$, $\mu > \sqrt{3}-1$. Our approach is a synthesis of earlier work and of new ideas. Global conditions on the potentials are imposed only to define the dynamics. Asymptotic completeness is derived from the fact that the mean square diameter of the system diverges like t^2 as $t \to \pm\infty$ for any orbit ψ_t which is separated in energy from thresholds and eigenvalues (a generalized version of Mourre's theorem involving only the tails of the potentials at large distances). We introduce new propagation observables which considerably simplify the phase–space analysis. As a topic of general interest we describe a method of commutator expansions.

0. INTRODUCTION

N-body quantum systems are described by the Schrödinger equation $i\partial_t\psi_t = H\psi_t$, with a Hamiltonian like

$$H = \sum_{k=1}^{N} \frac{p_k^2}{2m_k} + \sum_{i<k}^{1\ldots N} V_{ik}(x_i - x_k). \tag{0.1}$$

After fixing the center of mass H acts on the Hilbert space $\mathcal{H} = L^2(X)$, where

$$X = \{x = (x_1, \ldots, x_N) \mid x \in R^3;\ \sum m_k x_k = 0\}. \tag{0.2}$$

In general H possesses eigenvectors (stationary states), which span the subspace $\mathcal{H}_B$ of bound states where the orbits ψ_t are recurrent. In the continuous spectral subspace $\mathcal{H}_C = \mathcal{H}_B^\perp$ the long-time behaviour of ψ_t depends critically on the decay rate of the potentials, expressed by

$$V_{ik}(x_i - x_k) = O(|x_i - x_k|^{-\mu}) \qquad \text{as } |x_i - x_k| \to \infty .$$

If μ is not too small it is expected that along *any* orbit ψ_t in $\mathcal{H}_C$ the system eventually breaks up into a collection of almost freely moving, bound subsystems (fragments) as $t \to \pm\infty$. This is the conjecture of asymptotic completeness, which was stated precisely in the early days of scattering theory [Jauch], [Hack]. The challenge to prove this conjecture then became a driving force in the mathematical theory of N-body systems. New methods of spectral analysis and new tools to control the space-time propagation of quantum states gradually emerged over the last 30 years, often with results not directly related to scattering theory but important in their own right. As a culmination of these efforts Sigal and Soffer [SigSof1] in 1987 gave the first general proof of asymptotic completeness for short-range potentials ($\mu > 1$). Further insight and important simplifications came from the subsequent work of Graf [Graf1] and Yafaev [Yaf]. An approach to the qualitatively different long-range problem ($\mu \leq 1$) was initiated by Sigal and Soffer in their study of the Coulomb case [SigSof3–4]. With this starting point the long-range problem was solved by Dereziński [Der2] for $\mu > \sqrt{3} - 1$ and by Sigal and Soffer [SigSof5] for the Coulomb case ($\mu = 1$).

We briefly summarize the long history of the subject. A first milestone was Faddeev's solution of the 3-body problem using stationary methods (Faddeev equations [Fad]), later extended to all N [Hepp, Sig1]. This approach is used today for computational work on small systems, but its scope, especially for $N > 3$, is still limited by spectral assumptions on the subsystems (no eigenvalues embedded in the continuum, no resonances at thresholds). The Faddeev equations and their generalizations are designed to obtain the scattering amplitudes (S-matrix elements in p-space). Asymptotic completeness (unitarity of the S-matrix) emerges as a by-product at the end, thus offering little intuitive insight into the basic reasons for its validity.

The space-time point of view was primarily developed in quantum field theory under the influence of Haag [Haag1-2] and Ruelle [Rue1]. It regained attention in non–relativistic quantum mechanics after Ruelle's ergodic characterization of bound states vs. continuum states [Rue2] (RAGE Theorem, see e.g. [CFKS] or [HunSig]). Asymptotic completeness for N–body systems in the limit of weak forces was obtained by time–dependent perturbation methods ([Hun], [IorCar]). Positive commutators ([Put], [Kato2]) and related (global) propagation estimates first entered in Lavine's proof of asymptotic completeness for N–body systems with purely repulsive forces [Lav1-2]. The commutator in question is familiar from the virial theorem:

$$i[H,A] \;=\; \sum_k \frac{p_k^2}{m_k} - \sum_{i<k} (x_i - x_k)\cdot \nabla V_{ik}(x_i - x_k), \tag{0.3}$$

where

$$A \;=\; \sum_k \frac{1}{2}(x_k \cdot p_k + p_k \cdot x_k). \tag{0.4}$$

For repulsive forces the expression (0.3) is termwise positive. We also note that A is also the generator of the unitary group of dilations

$$e^{-iA\lambda}:\; \psi(x) \;\to\; e^{-\frac{\lambda}{2}\dim(X)}\psi(e^{-\lambda}x)$$

acting on $L^2(X)$, and that (0.3) is the infinitesimal form of the transformation law

$$e^{iA\lambda}\, H\, e^{-iA\lambda} \;=\; H(\lambda) \;:=\; e^{-2\lambda}\sum_k \frac{p_k^2}{2m_k} + \sum_{i<k} V_{ik}\big(e^{\lambda}(x_i - x_k)\big). \tag{0.5}$$

Moreover, A itself is a commutator, i.e.

$$A \;=\; i\Big[H,\, \frac{1}{2}\,x^2\Big], \qquad \text{where} \quad x^2 \;=\; \sum_k m_k x_k^2\,,$$

so that

$$\partial_t^2\, \langle \frac{1}{2}\,x^2\rangle_t \;=\; \partial_t\, \langle i[H,A]\rangle_t \;>\; 0\,. \tag{0.6}$$

Here $\langle \Phi\rangle_t \;=\; (\psi_t,\, \Phi\psi_t)$ denotes the expectation value of an observable Φ in the state ψ_t. (0.6) indicates that $\langle x^2\rangle_t$ diverges like t^2 as $t \to \pm\infty$, which holds in fact for a dense set of initial states ψ. A classical example is the case of Coulomb forces: then $i[H,A] = 2H - V \geq H$, where V is the total potential, and therefore

$$\langle x^2\rangle_t \;\geq\; \langle H\rangle \cdot t^2 \;+\; O(t) \;\to\; \infty \qquad (t \to \pm\infty).$$

At the same time and seemingly unrelated to the work of Lavine, Balslev and Combes [BalCom] determined the spectral properties of the operator family $H(\lambda)$ given by (0.5) *for complex* λ in the case of dilation-analytic potentials, thereby revealing the general nature of the essential spectrum of H (thresholds, embedded eigenvalues, absence of singular continuous spectrum) and laying the foundation of a theory of resonances [Sim1]. Further insight came from the geometric (configuration space) methods of spectral analysis and scattering theory developed in the later 1970's, e.g. in [Enss1], [Sim2], [DeiSim], [Sig2]). The most striking event of that time was Enss' proof that asymptotic completeness for $N = 2$ follows directly from Ruelle's Theorem combined with the propagation properties of *free wave packets* [Enss2]. Although the hope for a quick solution of the general case was premature, Enss' proof (and its later extensions to $N = 3$ in [Enss3–4]) marks the turning point to phase space analysis in N-body scattering theory.

Less noticed at first, and influenced by the work of Lavine and Balslev–Combes, Mourre [Mour1] introduced another key idea: For $N = 3$ he proved the *conditional positivity of the commutator (0.3) for forces of arbitrary sign*, in the sense that

$$E_\Delta(H) i[H, A] E_\Delta(H) \;\geq\; \theta E_\Delta(H) \tag{0.7}$$

(Mourre's inequality). Here $E_\Delta(H)$ is the spectral projection of H for an energy shell $\Delta = (E - \epsilon, E + \epsilon)$. If E is in the continuous spectrum of H, but not an eigenvalue nor a threshold, then (0.7) holds for sufficiently small $\epsilon > 0$ with a *strictly positive* θ. Mourre's inequality again leads to

$$\langle x^2 \rangle_t \;\geq\; \theta t^2 \;+\; O(t) \;\rightarrow\; \infty \qquad (t \rightarrow \pm\infty) \tag{0.8}$$

for a dense set of initial states in $\mathcal{H}_\Delta = \mathrm{Ran}\left(E_\Delta(H)\right)$. In fact (0.7) is a special case of a more general inequality given by Mourre, which holds for any $E \in R$, and which exhibits the structure of the essential spectrum of H in much the same way as dilation analyticity (of which it is an infinitesimal version). Mourre's inequality was soon extended to general

N by Perry, Sigal and Simon [PSS], who used it to derive the local decay estimate

$$\int_{-\infty}^{+\infty} \langle (1+x^2)^{-\alpha} \rangle_t \;\le\; C(\Delta,\alpha)\,\|\psi\|^2 \tag{0.9}$$

for $\alpha > 1/2$ and all ψ in $\mathcal{H}_\Delta$. For an exposition of these results we refer to [CFKS] and [HunSig].

Propagation estimates like (0.8) and (0.9) only say that the mean square diameter $\langle x^2 \rangle_t$ of the system diverges like t^2 as $t \to \pm\infty$. To demonstrate the break-up of the system into fragments (various scenarios of such break-ups are called the scattering channels), it is necessary to show that the probability for it to cross the phase-space boundaries of the channels is relatively small. More precisely, one proves estimates of the form

$$\int_{-\infty}^{+\infty} \|f(x,p)\psi_t\|^2 dt \;\le\; C(\Delta, f)\|\psi\|^2$$

for all ψ in $\mathcal{H}_\Delta$, where f is C_0^∞ in $p = (p_1, \ldots, p_N)$, smooth and homogeneous degree $-\frac{1}{2}$ for $|x| \ge 1$ in x and is supported outside the *classical* (phase-space) trajectories of *quantum* freely moving fragments for all possible break-ups. The latter is done by constructing observables which, unlike A, are H-bounded and have commutators with H positive in parts of the phase-space region one wants to control, but — and this is the price one has to pay — in general, negative elsewhere. The positive contributions lead to the desired propagation estimates, once the negative ones are controlled. A bootstrap type procedure allows to close the argument. This approach leaves room for different constructions, which are in fact the essence of every general proof of asymptotic completeness since the first proof by Sigal and Soffer, and this is where we claim to make a significant contribution.

Our paper is organized as follows. After the preliminaries on N–body systems and scattering theory (sections 1 and 2) we essentially follow Yafaev [Yaf] in constructing a function $g(x)$ on X which grows like $|x|$, but which incorporates the full channel structure of the system (given by the asymptotics of the total potential $V(x)$ as $x \to \infty$). Our propagation observables are derived from a modified and time–scaled Yafaev function

$$g_t(x) \;=\; t^\delta g(t^{-\delta}x)\,; \qquad 0 < \delta < 1\,, \tag{0.10}$$

or, in the Heisenberg picture, from the operator $g(t) = e^{iHt} g_t e^{-iHt}$. Its first derivative $\gamma(t) = \partial_t g(t)$ is bounded relative to H and *essentially increasing*: $\partial_t \gamma(t) \geq 0$ up to terms with an integrable time decay (section 3). This establishes the asymptotic observable

$$\gamma^+ = \underset{t\to\infty}{s\text{-lim}}\, \gamma(t) = \underset{t\to\infty}{s\text{-lim}}\, \frac{g(t)}{t} \geq 0 , \tag{0.11}$$

which commutes with H (section 4). Due to the special geometry of $g(x)$ it follows that any orbit ψ_t in the range of γ^+ is an outgoing scattering state:

$$\psi_t \longrightarrow \sum_a e^{-iH_a t} \phi_a \qquad (t \to +\infty) , \tag{0.12}$$

where a labels the channels and where H_a is the channel Hamiltonian describing independent fragments (section 5). To prove asymptotic completeness it then remains to show that the range of γ^+ is dense in the continuous spectral subspace $\mathcal{H}_C$ of H. This is where the Mourre inequality comes in. Since $g(x)$ grows like $|x|$, (0.8) and (0.11) lead to

$$\theta E_\Delta(H) \leq \liminf_{t\to\infty} E_\Delta(H) \frac{g^2(t)}{t^2} E_\Delta(H) = E_\Delta(H)(\gamma^+)^2 E_\Delta(H).$$

This shows that γ^+ reduces to a strictly positive operator $\mathcal{H}_\Delta \mapsto \mathcal{H}_\Delta$. By Mourre's Theorem the subspaces of $\mathcal{H}_\Delta$ span $\mathcal{H}_C$, so that $\mathrm{Ran}\,(\gamma^+)$ is indeed dense in $\mathcal{H}_C$.

This thumbnail sketch covers the short range case. The long range problem is qualitatively different. For reasons explained at the end of section 2, we want to deal from the outset with weakly time–dependent Hamiltonians of the form $H_t = H + W_t(x)$, where $W_t(x)$ decays like $(t+|x|)^{-\mu}$. The relation (0.11) extends easily to this more general setting, and (0.12) has a natural analogue on the range of γ^+ (sections 6 and 7). However, γ^+ no longer commutes with H, and there is no Mourre estimate for the dynamics generated by H_t since strict energy conservation is lost. The core of the long range problem is to link the states ψ with $\gamma^+\psi = 0$ to the bound states of H (section 8). The difficulty here is that the spectral support of ψ_t with respect to H cannot be separated from thresholds (outside of which the Mourre inequality holds) by initial conditions. This means that the minimal distance between the fragments cannot grow proportional to t. An inductive procedure reduces the problem of controlling such orbits to showing that if the diameter of the system grows as t^δ with $\delta < 1$ then the system is in a bound state. This was first done in [SigSof4] for $N \leq 4$ and in [Der2] for general N (see also [SigSof5]). The solution of this problem also allows an effortless proof of the existence of the long range wave operators (section 9). Finally, the extra propagation estimates needed in sections 8 and 9 are derived in Appendix C by a general method of commutator expansions, which is of independent interest (Appendix B). These estimates replace the Mourre inequality, or more precisely its consequence (0.8), in the case of time-dependent Hamiltonians.

1. N-BODY SYSTEMS

From the standard example (0.1) we extract the three basic constituents which in this paper characterize a N-body system: The configuration space X, the lattice L of channels and the intercluster potentials I_a. The resulting more general class of systems is the same as the one introduced by Agmon [Agm], but described from a somewhat different point of view.

Configuration Space. X is a Euclidean space with a scalar product denoted by $x \cdot y$. In the example (0.2):

$$x \cdot y \;=\; \sum_k m_k (x_k \cdot y_k)_{R^3}\,. \tag{1.1}$$

We note that $\frac{1}{2}(\dot{x} \cdot \dot{x}) = \frac{1}{2}\dot{x}^2$ is the classical kinetic energy and $p = \dot{x}$ the momentum conjugate to x. The Hamiltonian is of the form

$$H \;=\; \frac{1}{2}p^2 + V(x)\,. \tag{1.2}$$

In quantum mechanics this is an operator on $L^2(X)$, where $p = -i\nabla$ and $p^2 = -\Delta$ have their usual form in *cartesian coordinates* (not the particle coordinates) of X.

Channels. In X there is a distinguished finite lattice L of subspaces $a, b, \ldots$ (channels), which is closed under intersections and which contains $\{0\}$ and X. In the example (0.1) the channels correspond to all partitions of $(1 \ldots N)$ into subsets (clusters), e.g. if $N = 4$:

$$\text{partition}: \ (12)(34) \ \longleftrightarrow \ \text{channel}: \ a = \{x \in X \mid x_1 = x_2;\, x_3 = x_4\}. \tag{1.3}$$

In general we define the partial ordering of L by

$$a < b \ \leftrightarrow \ a \subset b, \ a \neq b\,. \tag{1.4}$$

For each $a \in L$ there is an orthogonal splitting

$$X \ = \ a \oplus a^{\perp}\,, \tag{1.5}$$

and we write the corresponding decomposition of a vector $x \in X$ as

$$x = x_a + x^a; \quad x_a \in a, \ x^a \in a^{\perp}\,. \tag{1.6}$$

The example (1.3) shows that x_a describes the CM– (center of mass) positions of the clusters and x^a the internal configuration of each cluster in its own CM-frame (Fig.1).

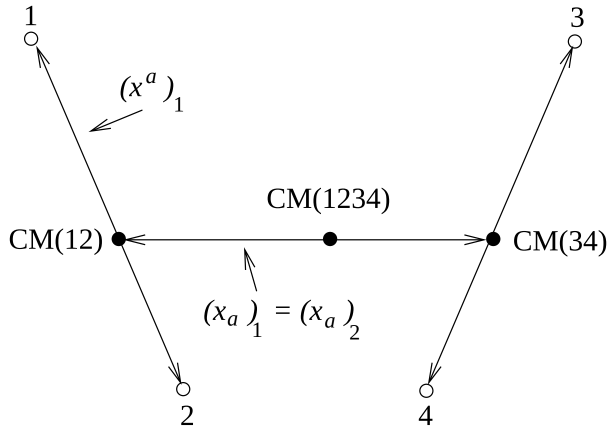

Fig. 1

Viewed as a map of configurations in R^3, the projection $x \to x_a$ sends each particle into the CM of its cluster, while $x \to x^a$ translates each cluster as a whole so that its CM is relocated at the origin.We note that

$$\frac{1}{2}\,p^2 = \frac{1}{2}(p_a)^2 + \frac{1}{2}(p^a)^2 \tag{1.7}$$

expresses the familiar decomposition of the kinetic energy into CM-parts and internal parts with respect to the clusters in the channel a.

Intercluster Distance. In the example (1.3) the spatial separation of the clusters in a given configuration x can be described by their distance as subsets of R^3, i.e. by

$$d_a(x) \;=\; \min_{i\in(12);\,k\in(34)} |x_i - x_k|. \tag{1.8}$$

However, it is more convenient to express the separation in terms of the geometry of X. Some reflection shows that

$$d_a(x) = 0 \;\Leftrightarrow\; x \in b,\; b\cap a < a\,. \tag{1.9}$$

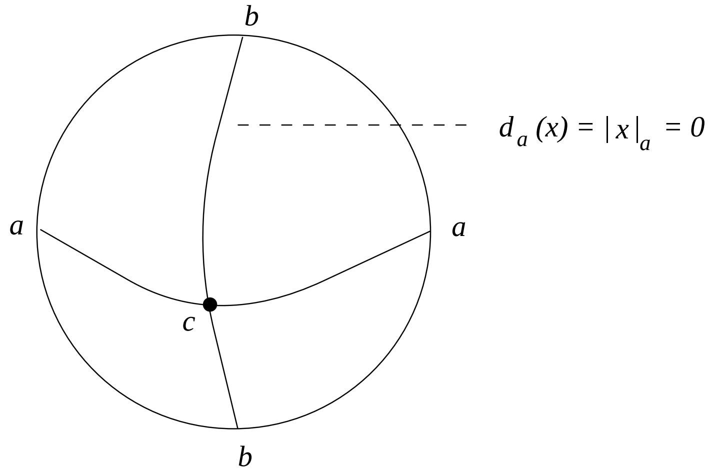

Fig. 2

Fig. 2 shows the unit sphere in X, intersected by two channels a, b with $a \cap b = c < a$. This motivates our general definition of the *intercluster distance*:

$$|x|_a \;:=\; \min_{b\cap a<a} |x^b|; \qquad a > \{0\}\,. \tag{1.10}$$

In the case (1.3) one finds

$$|x|_a \;=\; \min_{i\in(12);\,k\in(34)} \left(\frac{m_i m_k}{m_i + m_k}\right)^{\frac{1}{2}} |x_i - x_k|\,,$$

which serves as well as (1.8). We note that in general, for $a > \{0\}$,

$$a^* \ := \ a \setminus \bigcup_{c<a} c \ = \ \{ x \in X \mid |x|_a > 0 \}. \tag{1.11}$$

Intercluster Potentials. The basic fact about N-body systems is that for far separated clusters the potential depends only on the *internal configuration of the clusters.* To formulate this, let $a > \{0\}$ and $y \in a^*$. Then the translations

$$x \ \longrightarrow \ x + sy \qquad (s \in R)$$

do not affect x^a, while $|x+sy|_a \to \infty$ as $s \to \infty$. We therefore require that the limits

$$V^a(x^a) \ := \ \lim_{s\to\infty} V(x+sy) \tag{1.12}$$

exist and depend only on x^a. More precisely,

$$V(x) \ = \ V^a(x^a) + I_a(x)\,; \qquad I_a(x) \le f(|x|_a) \to 0 \text{ as } |x|_a \to \infty\,. \tag{1.13}$$

Our understanding is that the function $I_a(x)$ — called the *intercluster potential* — is only defined for $|x|_a > R$, where R is some arbitrary large constant. So, if we later impose similar conditions on certain derivatives of $I_a(x)$, this implies only that these derivatives exist for $|x|_a > R$. Also, if $I_a(x)$ (or a derivative of $I_a(x)$) appears as an operator acting on some state $\psi \in L^2(X)$, this state must be supported in $|x|_a > R$ else the expression is not defined. On the other hand the potentials $V^a(x^a)$ are defined by (1.12) for *all* $x^a \in a^\perp$. To complete the definition of V^a and I_a we set

$$I_{\{0\}}(x) = 0;\ V^{\{0\}}(x) = V(x) \quad \forall x,$$

and since V^X is just a constant we normalize $V(x)$ by setting

$$V^X = 0:\ I_X(x) = V(x) \ \text{ for } |x|_X > R\,.$$

In the example (1.3) we have

$$\begin{aligned} V^a &= V_{12} + V_{34} && (\forall\ x^a)\,; \\ I_a &= V_{13} + V_{14} + V_{23} + V_{24} && (|x|_a > R)\,; \end{aligned}$$

and in general, corresponding to $L^2(X) = L^2(a) \otimes L^2(a^\perp)$:

$$\begin{aligned} H &= H_a + I_a && (|x|_a > R)\,; \\ H_a &= \frac{1}{2}(p_a)^2 \otimes 1 + 1 \otimes H^a && \text{on } L^2(X)\,; \\ H^a &= \frac{1}{2}(p^a)^2 + V^a && \text{on } L^2(a^\perp)\,. \end{aligned} \tag{1.14}$$

H_a describes the dynamics of a system of non-interacting clusters and conserves p_a, H^a describes the internal dynamics of these clusters.

Conditions on the potential. First we need some global properties of V to make H (and in fact all the Hamiltonians (1.14)) self-adjoint and bounded from below. Further, it is essential that the kinetic energy is bounded by the total energy in form sense:

$$\langle\ p^2\ \rangle_\psi \ \le\ \text{const.}\ \langle\ H + c\ \rangle_\psi\,, \tag{1.15}$$

where c is some constant to make $H + c \ge 1$. To minimize domain considerations we make the working assumption that V is a *Kato-potential* : *For any* $\alpha > 0$ *there exists* $\beta < \infty$ *such that*

$$\|V\psi\| \ \le\ \alpha\|p^2\psi\| + \beta\|\psi\| \qquad \forall\ \psi \in C_0^\infty(X)\,. \tag{1.16}$$

Then H is self-adjoint on $D(p^2)$ and satisfies (1.15) [Kat1], [RSII]. We will not reiterate this assumption in the following. The reader who is interested in N-body systems with more general (even strongly singular) potentials should consult [Gri]. Since our topic is scattering theory, we concentrate on the fall-off of conditions for the intercluster potentials. These conditions are of the form

$$\partial_x^k I_a(x) \ =\ O(|x|_a^{-\mu-|k|}) \qquad (|x|_a \to \infty)\,, \tag{1.17}$$

in the sense of (1.13), where k a multi-index. We will state the relevant values of μ and $|k|$ for each step.

Induction Principle. To summarize, we have characterized N-body systems by three constituents:

$$\begin{aligned} &\text{– a configuration space } X \\ &\text{– a lattice } L \text{ of channels} \\ &\text{– a potential } V(x) \text{ satisfying (1.16), (1.13), (1.17).} \end{aligned} \tag{1.18}$$

In this sense each Hamiltonian H^a in (1.14) also describes a N-body system: its configuration space is $a^\perp$, its channels are the subspaces $b \cap a^\perp$, $b \geq a$, and its potential $V^a(x^a)$ is an offspring of $V(x)$ given by (1.12). It is an exercise to check that V^a inherits all the properties we have imposed on V [HunSig]. To derive some proposition $\mathcal{P}$ from (1.18) we can therefore use *induction on the lattice* L as follows. First, $\mathcal{P}$ is verified in the trivial case $a = X$: $H^X = 0$ on $L^2(\{0\}) = C$. Then $\mathcal{P}$ is proved for $a = \{0\}$: $H^{\{0\}} = H$, under the hypothesis that $\mathcal{P}$ holds for any H^a with $a > \{0\}$. An example will be our proof of asymptotic completeness.

2. SCATTERING STATES AND ASYMPTOTIC COMPLETENESS

Short range systems. ($\mu > 1$) Outgoing scattering states ψ are characterized by the asymptotic condition

$$\psi_t = e^{-iHt}\psi \underset{\|\,\|}{\longrightarrow} \sum_{a \in L} e^{-iH_a t}\varphi_a \qquad (t \to +\infty); \tag{2.1}$$

$$\varphi_a \in \mathcal{H}_a := L^2(a) \otimes \mathcal{H}_B(H^a)\,, \tag{2.2}$$

where $\mathcal{H}_B(H^a)$ is the subspace of $L^2(a^\perp)$ spanned by the eigenvectors of H^a. Each term in the sum (2.1) represents a free motion of bound clusters in the channel a. For convenience we have included the bound state channel $a = \{0\}$: if $\psi \in \mathcal{H}_B(H)$ then (2.1) holds trivially with $\varphi_{\{0\}} = \psi$, $\varphi_a = 0$ for $a > \{0\}$. The existence of a unique scattering state ψ for any given $\{\varphi_a\}$ is one of the earliest results in N–body scattering theory [Hack]: if $I_a(x) = O(|x|_a^{-\mu})$, $\mu > 1$, then the wave operators

$$\Omega_a^+ \; = \; s - \lim_{t \to +\infty} e^{iHt} e^{-iH_a t} \tag{2.3}$$

exist on $\mathcal{H}_a$, so that (2.1) holds for

$$\psi \; = \; \sum_a \Omega_a^+ \varphi_a \, . \tag{2.4}$$

The wave operators are isometric from $\mathcal{H}_a$ to $\mathcal{H}$. Moreover, their ranges $\mathcal{H}_a^+ = \mathrm{Ran}(\Omega_a^+)$ satisfy

$$\mathcal{H}_a^+ \perp \mathcal{H}_b^+ \qquad (a \neq b) \, , \tag{2.5}$$

expressing the fact that

$$\lim_{t \to +\infty} (e^{-iH_a t} \varphi_a, \; e^{-iH_b t} \varphi_b) \; = \; 0 \qquad (a \neq b) \; . \tag{2.6}$$

Therefore (2.4) is an orthogonal sum:

$$\|\psi\|^2 \; = \; \sum_a \|\Omega_a^+ \varphi_a\|^2 \; = \; \sum_a \|\varphi_a\|^2 \; , \tag{2.7}$$

and the outgoing scattering states form a *closed* subspace

$$\mathcal{H}^+ \; = \; \bigoplus_a \mathcal{H}_a^+ \; \subset \; \mathcal{H} \, . \tag{2.8}$$

The proofs of (2.3) and (2.6) involve only the propagation properties of free wave packets describing the center of mass motion (see e.g. [RSIII]). *Asymptotic completeness* is the statement that

$$\mathcal{H}^+ \; = \; \mathcal{H} \; , \tag{2.9}$$

which says that *any orbit* ψ_t of the system has the asymptotic form (2.1) as $t \to +\infty$, and therefore (by time reversal) also for $t \to -\infty$. The first main result we want to prove is

Theorem 2.1. *(Asymptotic completeness of short range systems) (2.9) holds if for some* $\mu > 1$

$$I_a(x) \;=\; O(|x|_a^{-\mu}) \quad \text{as } |x|_a \to \infty. \tag{2.10}$$

Remarks. This is the result first obtained by Sigal and Soffer [SigSof1] for a somewhat smaller class of potentials, and then successively by Graf [Graf1], Tamura [Tam] and Yafaev [Yaf]. Proofs under the sole condition (2.10) and allowing singular potentials were given by Iftimovici [Ift], Boutet de Monvel, Georgescu and Soffer [BoGeSo], and Griesemer [Gri]. See also [DerGer2].

Outline of the proof. An orbit ψ_t is called *asymptotically clustering* if

$$\psi_t \underset{\|\,\|}{\longrightarrow} \sum_a e^{-iH_a t}\varphi_a \qquad (t \to +\infty) \tag{2.11}$$

for *some* $\varphi_a \in \mathcal{H}$, i.e. without the condition (2.2). Again this is trivially true for $\psi \in \mathcal{H}_B(H)$. In section 5 we will prove asymptotic clustering for a *dense set* of orbits ψ_t. Then we invoke the induction hypothesis that asymptotic completeness holds for the systems described by H^a for all $a > \{0\}$, which is true for $a = X$. This is equivalent to saying that, for any $\varphi_a \in \mathcal{H}$,

$$e^{-iH_a t}\varphi_a \underset{\|\,\|}{\longrightarrow} \sum_{b \geq a} e^{-iH_b t}\varphi_{ab} \qquad (t \to \infty)\;; \qquad \varphi_{ab} \in L^2(b) \otimes \mathcal{H}_B(H^b)\;. \tag{2.12}$$

Inserting (2.12) into (2.11) gives

$$\psi_t \underset{\|\,\|}{\longrightarrow} \sum_b e^{-iH_b t} \sum_{a \leq b} \varphi_{ab} \qquad (t \to \infty)\,, \tag{2.13}$$

i.e. $\psi \in \mathcal{H}^+$. Since this holds for a dense set of ψ's and since $\mathcal{H}^+$ is closed it follows that $\mathcal{H}^+ = \mathcal{H}$.

Long range systems. ($\mu \leq 1$) For μ not too small the appropriate asymptotic condition generalizing (2.1) is of the form

$$e^{-iHt}\psi \underset{\|\,\|}{\longrightarrow} \sum_{a \in L} e^{-iH_a t - i\alpha_{a,t}(p_a)}\varphi_a \qquad (t \to \infty)\,, \tag{2.14}$$

with $\varphi_a \in L^2(a) \otimes H_B(H^a)$ as before. In other words: only the free center-of-mass propagator of the fragments in channel a is modified from

$$e^{-\frac{i}{2}p_a^2 t} \quad \text{to} \quad e^{-\frac{i}{2}p_a^2 t - i\alpha_{a,t}(p_a)}\,, \tag{2.15}$$

which still conserves the momentum p_a. Here $\alpha_t(p_a)$ is an adiabatic phase arising from the fact that (in a classical picture) the fragments are located at

$$x_a \;=\; p_a t\big(1 + O(t^{-\mu})\big) \qquad (t \to \infty)$$

so that

$$I_a(x) \;=\; I_a(p_a t) + O(t^{-2\mu}) \tag{2.16}$$

provided that $\nabla I_a(x) = O(|x|_a^{-\mu-1})$ as $|x|_a \to \infty$. For $2\mu > 1$ the error term in (2.16) decays integrably in time, while the leading term is of order $t^{-\mu}$ and therefore not integrable if $\mu \leq 1$. According to this classical picture the Ansatz

$$\alpha_{a,t}(p_a) \;=\; \int^t ds\, I_a(p_a s) \tag{2.17}$$

should work for $\mu > \frac{1}{2}$. The reason why we have not fully defined $\alpha_{a,t}(p_a)$ is twofold. First, it is clear that the modified propagator (2.15) is insensitive to a change of $\alpha_{a,t}(\cdot)$ on a null set of a. This allows us to restrict p_a to the set a^* (1.11), where $I_a(p_a s)$ indeed decays like $s^{-\mu}$. Secondly, $\alpha_{a,t}(p_a)$ is arbitrary within gauge transformations of the kind

$$\alpha_{a,t}(p_a) \longrightarrow \alpha_{a,t}(p_a) + f_t(p_a) \tag{2.18}$$

if $\lim\limits_{t\to\infty} f_t(p_a) = f_\infty(p_a)$ exists, since in (2.14) the phase $f_\infty(p_a)$ can be absorbed in φ_a. This is why the integrable error in (2.16) has no effect and why (2.14) is equivalent to (2.1) if $\mu > 1$. A complete definition of $\alpha_{a,t}(p_a)$ modulo gauge transformations is therefore

$$\alpha_{a,t}(p_a) \;=\; \int_{R|p_a|_a^{-1}}^t ds\, I_a(p_a s) \qquad (p_a \in a^*)\,, \tag{2.19}$$

if for $|x|_a > R$

$$|I_a(x)| \;\leq\; \text{const.}\, |x|_a^{-\mu}\,; \qquad |\nabla I_a(x)| \;\leq\; \text{const.}\, |x|_a^{-\mu-1}\,. \tag{2.20}$$

For $a = \{0\}$ we have $p_a = 0$ and we set $\alpha_{\{0\},t} = 0$. An important example is a system of charged particles (the Coulomb case). Then for $p_a \in a^*$

$$I_a(p_a t) \;=\; t^{-1} \sum_{\alpha<\beta} e_\alpha e_\beta \left| \frac{p_\alpha}{m_\alpha} - \frac{p_\beta}{m_\beta} \right|^{-1}\,, \tag{2.21}$$

where the sum runs over all *pairs of clusters* in the channel a with (total) charges e_α, masses m_α and momenta $p_\alpha \in R^3$. A corresponding phase $\alpha_{a,t}(p_a)$ is simply obtained by changing the factor t^{-1} to $\log(t)$. (This phase differs from (2.19) by a gauge transformation.) The formulas (2.1)–(2.9) can now be transcribed to the long-range case simply by replacing

$$H_a \longrightarrow H_a + \alpha_{a,t}(p_a)\,. \tag{2.22}$$

The proof of the existence of Ω_a^+ is considerably more difficult. In fact the first proofs for general N without *ad hoc* assumptions on the decrease of bound state wave functions at infinity appeared as by–products of proofs of asymptotic completeness ([Der2],[Ziel]). For the same reason we defer the proof to section 9. The second main result we prove is

Theorem 2.2. *(Asymptotic completeness of long range systems) (2.9) holds if for some* $\mu > \sqrt{3} - 1$ *and* $0 \leq |k| \leq 2$

$$\partial_x^k I_a(x) \;=\; O(|x|_a^{-\mu-|k|}) \quad \text{as } |x|_a \to \infty. \tag{2.23}$$

Remark. This is the result first obtained by Dereziński [Der2] under somewhat stronger conditions on the potentials. The borderline $\mu = \sqrt{3} - 1$ was identified by Enss for $N = 3$ [Enss4] and is further discussed in [Der1]. Another proof is due to Zielinski [Ziel]. See also [DerGer2].

The proof of Theorem 2.2 will be given in sections 6–8. At this point we only remark that the simple induction scheme given above in the short-range case does not work in the long-range case. Proceeding inductively, we will encounter time-dependent Hamiltonians similar to (2.22), acting on fibers of constant $p_a \in a^*$. This suggests an inductive proof for more general Hamiltonians of the form $H_t = H + W_t(x)$ (Theorem 6.2). The special case of Theorem 2.2 is then obtained by setting $W_t(x) \equiv 0$ *after performing the induction.*

3. YAFAEV FUNCTIONS AND THE BASIC PROPAGATION ESTIMATE

All our propagation observables are descendants of a time-scaled multiplication operator

$$g_t(x) \;=\; t^\delta g(t^{-\delta}x)\,; \qquad 0<\delta<1\,, \tag{3.1}$$

defined for $t>0$, where $g(x)$ is a positive smooth function on X with the same growth as $|x|$:

$$0 \;<\; c_1|x| \;\le\; g(x) \;\le\; c_2|x| \quad (|x|\ge 1). \tag{3.2}$$

Therefore the Mourre estimate (0.8) is equivalent to

$$\liminf_{t\to\infty} \left\langle \frac{g_t^2}{t^2} \right\rangle_t \;\ge\; \theta\,, \tag{3.3}$$

for some $\theta > 0$ and for the same orbits ψ_t. Unlike $|x|$, however, $g(x)$ will be carefully adapted to the lattice of channels. In this construction we essentially follow Yafaev [Yaf], who was motivated by a similar construction of Graf [Graf1]. To explain the requirements we formally compute the Heisenberg derivatives

$$\begin{aligned} \gamma_t \;&:=\; D_t g_t \;:= i[H,g_t] + \partial_t g_t \\ &=\; \frac{1}{2}\big(\nabla_{g_t}\cdot p + p\cdot\nabla_{g_t}\big) + \partial_t g_t; \end{aligned} \tag{3.4}$$

$$D_t(\gamma_t - 2\partial_t g_t) \;=\; p g_t'' p - i[\gamma_t, V] - \frac{1}{4}\,\Delta^2 g_t - \partial_t^2 g_t\,. \tag{3.5}$$

Here $g_t''(x)$ is the Hessian of $g_t(x)$ and (in cartesian coordinates)

$$p g_t'' p \;=\; \sum_{ik} p_i\,\frac{\partial^2 g_t}{\partial x_i \partial x_k}\,p_k\,. \tag{3.6}$$

We will call g a *Yafaev function* if it satisfies the conditions (Y.1) and (Y.2) given below.

Condition (Y.1). *g is a smooth, strictly positive convex function on X, constant for $|x| < R^-$, and homogeneous of degree 1 for $|x| > R^+$ ($0 < R^- < R^+$ arbitrary).*

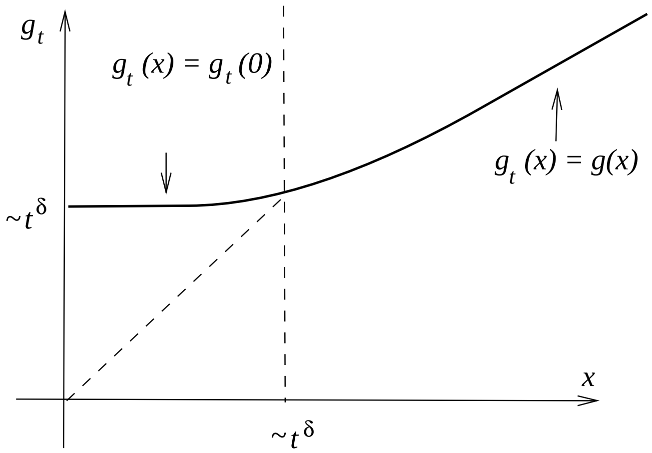

Fig. 3

A radial section of the scaled function g_t is shown in Fig. 3. We note that for $t \to \infty$

$$\partial_x^k g_t(x) \;=\; O(t^{\delta(1-|k|)}); \qquad \partial_t^k g_t(x) \;=\; O(t^{\delta-k}) \tag{3.7}$$

uniformly in x. In particular, ∇g_t is bounded uniformly in (x,t) and supported in $|x| > t^\delta R^-$, while $\partial_t g_t$ is supported in $|x| < t^\delta R^+$ and bounded by const.$t^{\delta-1}$. By (1.15) γ_t is defined on $D(|p|)$ and satisfies a uniform estimate

$$\|\gamma_t\psi\| \;\leq\; \text{const.}\langle\, H + c\,\rangle_\psi^{1/2} \qquad \forall\psi \in D(|p|). \tag{3.8}$$

(3.5) is understood in form sense on $D(|p|)$. The last two terms are bounded and of order

$$\frac{1}{2}\Delta^2 g_t \;=\; O(t^{-3\delta}); \quad \partial_t^2 g_t \;=\; O(t^{\delta-2}) \tag{3.9}$$

uniformly in x as $t \to \infty$. The term $pg_t''p$ is positive due to the convexity of g and decays only like $t^{-\delta}$:

$$0 \;\leq\; pg_t''p \;\leq\; \text{const.}t^{-\delta}(H + c)\,. \tag{3.10}$$

To treat the commutator $i[\gamma_t, V]$ we impose the further condition

Condition (Y.2). *For any $a > \{0\}$, $g(x) = g(x_a)$ on some cone C_a (invariant under $x \to \lambda x$) containg some set $\{x \mid |x^a| \le \varepsilon_a |x|,\ \varepsilon_a > 0\}$. Moreover, the cones C_a satisfy*

$$C_a \cap C_b \subset C_{a \cap b} \qquad \textit{for} \quad a \cap b < a, b\,. \tag{3.11}$$

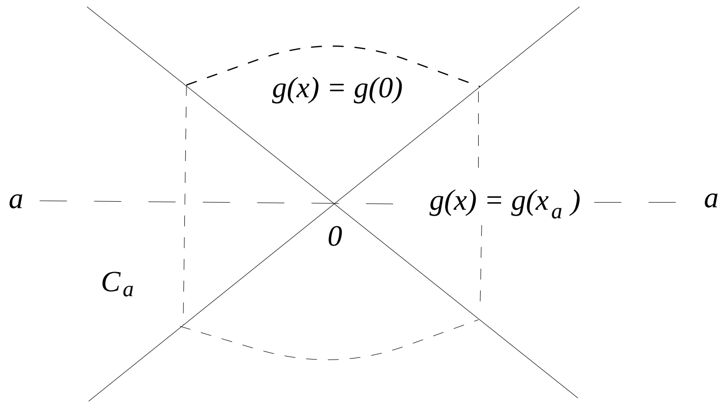

Fig. 4

Fig. 4 shows a cone C_a, intersected with the compact set where $g(x) = g(0)$.

Lemma 3.1. *The sets*

$$C_a^* \ := \ C_a \setminus \bigcup_{b<a} C_b$$

form a disjoint covering of X. Also

$$C_b \cap C_a^* \ = \ \phi \qquad \textit{if } b \cap a < a\,, \tag{3.12}$$

$$\textit{and} \quad |x|_a \ \ge \ |x| \cdot \min_{b \cap a < a} (\varepsilon_b) \quad \textit{for} \quad x \in C_a^*\,. \tag{3.13}$$

Proof. The first statement follows from $C_X = X$ and (3.11). Let $b \cap a < a$ and $x \in C_b \cap C_a^*$. This excludes $b \ge a$ and $b < a$. But $b \cap a < a, b$ is equally excluded since then $x \in C_{a \cap b}$. Therefore if $x \in C_a^*$ then $|x^b| \ge \varepsilon_b |x|$ for $b \cap a < a$. □

On $C_a^* \cap \operatorname{supp}(\nabla g_t)$ we thus have

$$\nabla g_t(x) \in a; \quad \text{and} \quad |x|_a \ \ge \ \lambda |x| \ \ge \ t^\delta \lambda R^- \tag{3.14}$$

for some $\lambda > 0$. If t is sufficiently large we can therefore decompose $V(x) = V^a(x^a) + I_a(x)$ in this region, which formally gives

$$i[\gamma_t, V] \;=\; \nabla g_t \cdot \nabla I_a(x)$$

since $\nabla g_t \cdot \nabla V^a = 0$. In the long-range case (Theorem 2.2) we have assumed that $\nabla I_a(x) = O(|x|_a^{-\mu-1})$, so that by (3.14)

$$|\nabla g_t \cdot \nabla I_a| \;\leq\; \text{const.}\, t^{-\delta(\mu+1)}$$

on each C_a^*. Since these sets cover X this estimate *holds globally* on X: for t sufficiently large

$$\big|(\psi, [\gamma_t, V]\psi)\big| \;\leq\; \text{const.}\, t^{-\delta(\mu+1)} \|\psi\|^2 \quad \forall\psi. \tag{3.15}$$

In the short range case we use $|I_a(x)| \leq \text{const.}\, |x|_a^{-\mu}$, which gives $|I_a(x)| \leq \text{const.}\, t^{-\delta\mu}$ on $\operatorname{supp}(\nabla g_t) \cap C_a^*$ for t sufficiently large. Therefore

$$\big|(\psi, [\gamma_t, V]\psi)\big| \;=\; 2\big|\operatorname{Im}(\gamma_t\psi, I_a\psi)\big| \;\leq\; \text{const.} t^{-\delta\mu}\langle H + c\rangle_\psi \tag{3.16}$$

for $\psi \in D(|p|)$ with support in C_a^*. This local estimate is independent of a and can be extended to all $\psi \in D(|p|)$ by using a suitable partition of unity (the sets C_a^* do not form an open covering of X, but they can be marginally enlarged to open sets for which (3.16) prevails). Collecting these results we have in form sense for sufficiently large t:

$$\begin{aligned} p g_t'' p \;&=\; D_t(\gamma_t - 2\partial_t g_t) + R_t\,; \\ |\langle R_t\rangle_\psi| \;&\leq\; \text{const.}\, t^{-\rho}\langle H + c\rangle_\psi \qquad \forall\psi \in D(|p|); \end{aligned} \tag{3.17}$$

provided that

$$\text{either}: \qquad I_a = O(|x|_a^{-\mu}) \qquad \text{and} \quad \rho \;=\; \min(\delta\mu, 3\delta, 2-\delta) \tag{3.18}$$

$$\text{or}: \qquad \nabla I_a = O(|x|_a^{-\mu-1}) \quad \text{and} \quad \rho \;=\; \min(\delta(\mu+1), 3\delta, 2-\delta) \tag{3.19}$$

Theorem 3.2. *Suppose that (3.17) holds for some $\rho > 1$. Then*

$$\int_1^\infty dt\, \langle p g_t'' p\rangle_t \;\leq\; \text{const.}\, \langle H + c\rangle_\psi \qquad \forall\psi \in D(|p|). \tag{3.20}$$

Proof. By (3.10) it suffices to consider the integral over an interval $t_0 < t < \infty$ where (3.17) holds. Integrating (3.17), and using the fact that $\gamma_t - 2\partial_t g_t$ is bounded relative to $|p|$ uniformly in t, we obtain

$$\int_{t_0}^{T} dt \langle p g_t'' p \rangle_t \;=\leq\; \text{const.} \langle H + c \rangle_\psi$$

uniformly in T. Since the integrand is positive, the limit $T \to \infty$ exists. □

Construction of $g(x)$. The prototype of $g(x)$ is

$$\widehat{g}(x, \sigma) \;=\; \max_{a \in L} f_a(x, \sigma)\,, \tag{3.21}$$

where $f_{\{0\}}(x, \sigma) = \sigma_{\{0\}}$ and $f_a(x, \sigma) = \sigma_a |x_a|$ for $a > \{0\}$. Here $\sigma = \{\sigma_a\}$ is a positive, decreasing function on the lattice L, to be adjusted in the course of the construction:

$$\sigma_{\{0\}} > \sigma_a > \sigma_b > \sigma_X > 0 \qquad \text{for} \;\; \{0\} < a < b < X\,. \tag{3.22}$$

$\widehat{g}(x, \sigma)$ is convex, constant on a compact set K containing some ball $|x| < R^-$, and homogeneous of degree 1 in the complement of K. $\widehat{g}$ has a decomposition into maximal pieces:

$$\begin{aligned} \widehat{g}(x, \sigma) \;&=\; \sum_a \widehat{g}_a(x, \sigma) \qquad \text{(a.e.)}\;; \\ \widehat{g}_a(x, \sigma) \;&=\; f_a(x, \sigma) \theta\big[f_a(x, \sigma) - \widehat{g}(x, \sigma)\big]\,, \end{aligned} \tag{3.23}$$

where θ is the characteristic function of $[0, \infty)$. The piece $\widehat{g}_{\{0\}}$ has support K where $\widehat{g}(x, \sigma) = \sigma_{\{0\}}$. The pieces $\widehat{g}_a$ for $a > \{0\}$ have conical supports where $\widehat{g}(x, \sigma) = \sigma_a |x_a|$. The intersection of these cones with a sphere of radius R^+ containing K is shown in Fig. 5:

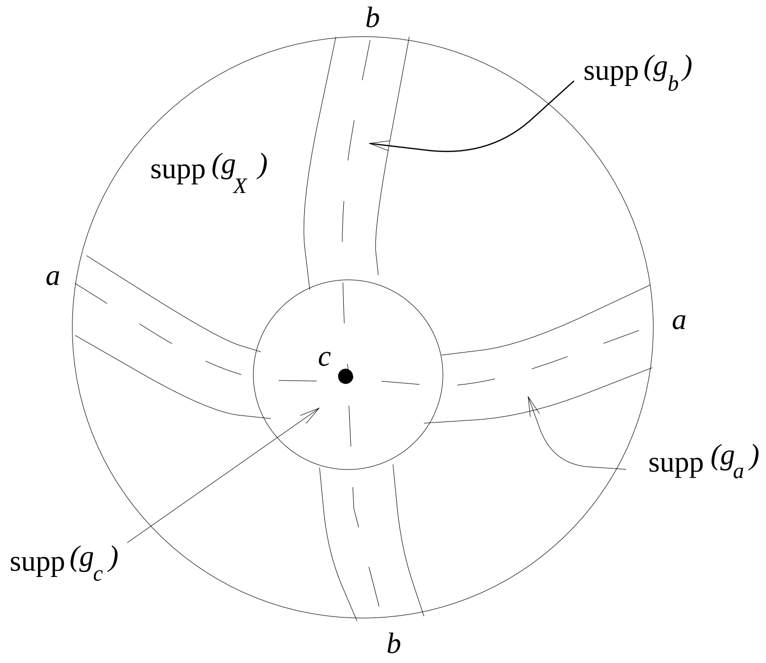

Fig. 5

This picture corresponds to Fig. 2 and serves to explain the choice of σ. To begin with suppose that $\sigma_a = \sigma_b = \sigma_c = 1$. Then Fig. 4 reduces to Fig. 2 since $|x_a| = |x|$ exactly if $x \in a$, etc. The situation of Fig. 5 is obtained by first increasing σ_a, σ_b (so that the supports of $\widehat{g}_a, \widehat{g}_b$ expand into strips), and then σ_c sufficiently far beyond σ_a, σ_b (such that $\mathrm{supp}\, \widehat{g}_c$ covers the intersection of the two strips). This corresponds to (3.11) and (3.12): in Fig. 5 the set C_a^* is just the support of $\widehat{g}_a$ where evidently

$$|x|_a \;\geq\; \lambda R \;(\lambda > 0) \quad \text{and} \quad \nabla g \in a\,,$$

except at boundary points where ∇g is discontinuous. This discontinuity is removed by a regularisation $\widehat{g}(x,\sigma) \to g(x)$ which preserves convexity:

$$g(x) \;=\; \int \widehat{g}(x,\mu) \prod_a \widetilde{\delta}(\mu_a - \sigma_a) d\mu_a\,, \tag{3.24}$$

where $0 \leq \widetilde{\delta} \in C_0^\infty(R)$ is a regularized Dirac distribution with arbitrary narrow support. The same regularisation is applied to $\widehat{g}_a(x,\sigma)$ so that

$$g(x) \;=\; \sum_{a \in L} g_a(x)\,. \tag{3.25}$$

The analytic construction of g is given in Appendix A. Here we summarize the relevant results:

Lemma 3.3. *g satisfies the conditions (Y.1) and (Y.2). Moreover g has a decomposition (3.25) into smooth functions g_a which have the following properties: There exists $\lambda > 0$ such that*

$$\mathrm{supp}(g_{\{0\}}) \;\subset\; \{x \mid |x| < R^+\}\,; \tag{3.26}$$

$$\mathrm{supp}(g_a) \;\subset\; \{x \mid |x|_a \geq \lambda|x| \geq \lambda R^-\} \quad \forall a > \{0\}\,; \tag{3.27}$$

$$\nabla g_{\{0\}}(x) \;=\; 0 \quad \text{for } |x| < R^-\,; \tag{3.28}$$

$$\nabla g_a(x) \;\in\; b \quad \text{for } x \in C_b\,, \quad \forall b > \{0\}\,. \tag{3.29}$$

The functions g_a are not convex. However, for any $a \in L$ there exists a Yafaev function $\widetilde{g}$ such that the Hessians of g_a and $\widetilde{g}$ satisfy

$$\pm g_a''(x) \;\leq\; \widetilde{g}''(x) \quad \forall x\,. \tag{3.30}$$

4. THE ASYMPTOTIC OBSERVABLE γ^+

Corresponding to (3.25) we set

$$g_t \;=\; \sum_a g_{a,t} \quad : \quad g_{a,t}(x) \;=\; t^\delta g_a(t^{-\delta}x)\,; \tag{4.1}$$

$$\gamma_t \;=\; \sum_a \gamma_{a,t} \quad : \quad \gamma_{a,t} \;=\; D_t g_{a,t}\,. \tag{4.2}$$

We also introduce the Heisenberg observables

$$g(t) \;=\; e^{iHt} g_t e^{-iHt}\,; \quad \gamma(t) \;=\; e^{iHt}\gamma_t e^{-iHt} \;=\; \partial_t g(t)\,, \tag{4.3}$$

and similarly for $g_a(t)$, $\gamma_a(t)$. The operator $\gamma(t)$ is defined on $D(|p|)$, both the operators $\gamma(t)$ and $g(t)$ on the domain $D(|x|) \cap D(|p|)$, which is invariant under $\exp(-iHt)$.

Theorem 4.1. *Under the hypothesis of Theorem 3.2 the strong limits*

$$\gamma^+ \;=\; \operatorname*{s\text{-}lim}_{t\to\infty}\gamma(t)\,; \qquad \gamma_a^+ \;=\; \operatorname*{s\text{-}lim}_{t\to\infty}\gamma_a(t) \tag{4.4}$$

exist on $D(|p|)$ and have the following properties:

$$[\gamma^+, H] \;=\; 0\,; \tag{4.5}$$

$$\gamma^+ \;=\; \operatorname*{s\text{-}lim}_{t\to\infty}\frac{1}{t}\,g(t) \;\geq\; 0 \tag{4.6}$$

on $D(|x|)\cap D(|p|)$, and similarly for γ_a^+. In particular

$$\gamma_{\{0\}}^+ \;=\; 0\;; \quad \text{i.e.} \quad \gamma^+ \;=\; \sum_{a>\{0\}}\gamma_a^+\,. \tag{4.7}$$

Moreover, γ^+ and γ_a^+ are independent of δ within the ranges allowed by the hypothesis of Theorem 3.2, since

$$\gamma^+ \;=\; \operatorname*{s\text{-}lim}_{t\to\infty} e^{iHt}\,\frac{g}{t}\,e^{-iHt} \qquad \text{on } D(|x|)\cap D(|p|)\,, \tag{4.8}$$

where g is the unscaled Yafaev function $g(x)$ (and similarly for γ_a^+).

Proof. Step (1): Existence of γ^+. By (3.8) it suffices to prove strong convergence of γ_t on the range of $(H+c)^{-2}$. First we show that

$$\operatorname*{s\text{-}lim}_{t\to\infty} e^{iHt}\,\gamma_t\,e^{-iHt}(H+c)^{-2} \;=\; \operatorname*{s\text{-}lim}_{t\to\infty}(H+c)^{-1}e^{iHt}\,\gamma_t\,e^{-iHt}(H+c)^{-1} \tag{4.9}$$

if one of these limits exists. Since $\|\partial_t g_t\| = O(t^{\delta-1})$ we can replace γ_t by $\gamma_t - \partial_t g_t$. Then (4.9) follows since

$$i[H, \gamma_t - \partial_t g_t] \;=\; p g_t'' p - \frac{1}{4}\,\Delta^2 g_t - i[\gamma_t, V]\,, \tag{4.10}$$

so that by our previous estimates

$$\|\,[\gamma_t - \partial_t g_t, (H+c)^{-1}]\,\| \;\to\; 0\,.$$

To establish the second limit in (4.9) it suffices to prove convergence of

$$\varphi_t \;=\; (c+H)^{-1} e^{iHt} \widetilde{\gamma}_t e^{-iHt} (c+H)^{-1} \psi$$

for all $\psi \in \mathcal{H}$, where we have chosen $\widetilde{\gamma}_t := \gamma_t - 2\partial_t g_t$. Then

$$\partial_t \varphi_t \;=\; (H+c)^{-1} e^{iHt} (D_t \widetilde{\gamma}_t) e^{-iHt} (H+c)^{-1} \psi\,, \tag{4.11}$$

and we show that this is strongly integrable. By (3.5) and by our previous estimates

$$D_t \widetilde{\gamma}_t \;=\; p g_t'' p$$

modulo terms which give integrable contributions.So it remains to prove that

$$u_t \;:=\; (H+c)^{-1} e^{iHt} p g_t'' p\, e^{-iHt} (H+c)^{-1} \psi$$

is strongly integrable over some interval $t_0 < t < \infty$. Factorizing the positive operator $pg_t''p$ into $pg_t''p \;=\; B_t^2\,;\;\; B_t = B_t^*$, we use the Schwarz inequality twice to estimate

$$\begin{aligned}
&\left\| \int_{t_1}^{t_2} dt\, u_t \right\|^2 \;=\; \sup_{\|v\|=1} \left| \int_{t_1}^{t_2} dt\, (v, u_t) \right|^2 \\
&\leq \sup_{\|v\|=1} \left(\int_{t_1}^{t_2} dt\, \|B_t e^{-iHt} (H+c)^{-1} v\|\, \|B_t e^{-iHt} (H+c)^{-1} \psi\| \right)^2 \\
&\leq \sup_{\|v\|=1} \int_{t_1}^{t_2} dt\, \|B_t e^{-iHt} (H+c)^{-1} v\|^2 \times \int_{t_1}^{t_2} dt\, \|B_t e^{-iHt} (H+c)^{-1} \psi\|^2 .
\end{aligned} \tag{4.12}$$

By Theorem 3.2 the first factor is bounded uniformly in t_1, t_2, and the second factor vanishes as $t_{1,2} \to \infty$.

Step (2): Existence of γ_a^+. This is proved in the same way with two notable differences. Instead of $i[\gamma_t, V]$ we encounter the commutator $i[\gamma_{a,t}, V]$, formally given by

$$i[\gamma_{a,t}, V] \;=\; \nabla g_{a,t} \cdot \nabla V\,.$$

This commutator is estimated like $i[\gamma_t, V]$ using (3.29). Secondly, since g_a is not convex $pg_{a,t}''p$ is not positive. Therefore we use the estimate (3.30) to split $pg_{a,t}''p$ into positive and negative parts:

$$p g_{a,t}'' p \;=\; A_t^+ - A_t^-\,; \quad \text{with} \quad 0 \leq A_t^{\pm} \leq p \widetilde{g}_t'' p\,.$$

Treating the contributions from $A_t^{\pm}$ separately, we then factorize $A_t^{\pm} = (B_t^{\pm})^2$ and use the propagation estimate (3.20) for $\widetilde{g}_t$.

Step (3): Properties of γ^+, γ_a^+. Since γ^+ exists it follows from (4.9) that

$$\gamma^+(H+c)^{-2} \;=\; (H+c)^{-1}\gamma^+(H+c)^{-1}\,,$$

i.e. $[\gamma^+, H] = 0$ (and similarly for γ_a^+). Using that $\gamma(t) = \partial_t g(t)$ we have on $D(|x|)\cap D(|p|)$:

$$\gamma^+ \;=\; \underset{t\to\infty}{s\text{-lim}}\,\frac{1}{t}\int_1^t ds\,\partial_s g(s) \;=\; \underset{t\to\infty}{s\text{-lim}}\,\frac{1}{t}\,g(t) \;\geq\; 0\,.$$

and similarly for γ_a^+. In particular

$$\gamma_{\{0\}}^+ \;=\; \underset{t\to\infty}{s\text{-lim}}\,\frac{1}{t}\,g_{\{0\}}(t) \;=\; 0$$

since $\|g_{\{0\}}(t)\| \leq \text{const.}\,t^{\delta}$. (4.8) follow from (4.6) and from the fact that

$$\frac{1}{t}\,\|g_t - g\| \;\leq\; \text{const.}\,t^{\delta-1}\;,$$

since $g_t(x) - g(x) = 0$ for $|x| \geq \text{const.}\,t^{\delta}$. $\square$

Next we discuss the connection between γ^+ and Mourre's inequality. In addition to (4.2) we introduce the Heisenberg observable

$$x^2(t) \;=\; e^{iHt}x^2e^{-iHt} \tag{4.13}$$

as a form on $D(|x|)\cap D(|p|)$. This domain is not only invariant under $\exp(-iHt)$, but also (via Fourier transform) under $f(H)$ for all $f \in C_0^{\infty}(R)$. Let $\Delta \subset R$ be a finite interval and let $\mathcal{H}_\Delta$ be the corresponding spectral subspace of H. Since γ^+ commutes with H and is bounded relative to H it reduces to a bounded symmetric operator $\mathcal{H}_\Delta \to \mathcal{H}_\Delta$. For the following Lemma we normalize $g(x)$ such that

$$|x| \;\leq\; g(x)\,. \tag{4.14}$$

Lemma 4.2. *Let $\Delta \subset R$ be an open finite interval in which H satisfies a Mourre estimate in form sense on D:*

$$\liminf_{t\to\infty} f(H)\,\frac{x^2(t)}{t^2}\,f(H) \;\geq\; \theta f^2(H) \quad (\theta > 0) \tag{4.15}$$

for all $f \in C_0^\infty(H)$. Then

$$\gamma^+ \;\geq\; \sqrt{\theta} \qquad \text{on } \mathcal{H}_\Delta\,, \tag{4.16}$$

in particular

$$\mathcal{H}_\Delta \;\subset\; \mathrm{Ran}(\gamma^+)\,. \tag{4.17}$$

On the other hand, if ψ is an eigenvector of H, then

$$\gamma^+\psi \;=\; 0\,. \tag{4.18}$$

Proof. Since $x^2(t) \leq g^2(t)$ we obtain from (4.15) and (4.6)

$$\theta f^2(H) \;\leq\; \liminf_{t\to\infty} f(H)\,\frac{g^2(t)}{t^2}\,f(H) \;=\; (\gamma^+)^2 f^2(H)$$

for all $f \in C_0^\infty(\Delta)$, which is equivalent to (4.16). If ψ is an eigenvector of H then

$$\|\gamma(t)\psi\| \;=\; \|\gamma_t\psi\|\,,$$

and we observe that $\gamma_t\psi \to 0$ since $\|\partial_t g_t\| \to 0$ and $\nabla g_t(x) = 0$ for $0 \leq |x| \leq R^- t^\delta$. □

We now quote the relevant parts of Mourre's Theorem in a generalized version due to Skibsted [Skib]. A simple proof inspired by Graf [Graf2] is given in [Gri]. See also [AmBoGe].

Theorem 4.3. *Suppose that*

$$\text{either}: \qquad \lim_{|x|_a\to\infty} |x|_a I_a(x) \;=\; 0\,; \tag{4.19}$$

$$\text{or}: \qquad \lim_{|x|_a\to\infty} |x|_a \nabla I_a(x) \;=\; 0\,. \tag{4.20}$$

Then the set $S \subset R$ given by

$$S \;=\; \bigcup_{a \in L} \{\textit{eigenvalues of } H^a\} \tag{4.21}$$

is closed and countable. For any $E \in R \backslash S$ there exists an open interval $\Delta \subset R \backslash S$, $\Delta \ni E$, and a constant $\theta > 0$ such that the Mourre inequality (4.15) holds.

Corollary 4.3.

$$\mathcal{H}_C(H) \;=\; \overline{\mathrm{Ran}(\gamma^+)}\,; \qquad \mathcal{H}_B(H) \;=\; \mathrm{Ker}(\gamma^+)\,. \tag{4.22}$$

Proof. Since S is countable and contains the eigenvalues of $H = H^{\{0\}}$, the spectral subspace of H corresponding to S is $\mathcal{H}_B(H)$. By Mourre's Theorem and (4.17), any state ψ with compact spectral support $\subset R \backslash S$ is in $\mathrm{Ran}(\gamma^+)$. This implies $\mathcal{H}_C(H) \subset \overline{\mathrm{Ran}(\gamma^+)}$. On the other hand it follows from (4.18) that $\mathcal{H}_B(H) \subset \mathrm{Ker}(\gamma^+)$. Since γ^+ is selfadjoint (4.22) follows. □

5. THE SHORT RANGE CASE

Theorem 5.1. *If $I_a(x) = O(|x|_a^{-\mu})$, $\mu > 1$, then the Deift-Simon wave operators*

$$\omega_a^+ \;=\; \operatorname*{s\text{-}lim}_{t \to \infty} e^{iH_a t} \gamma_{a,t} e^{-iHt} \tag{5.1}$$

exist on $D(|p|)$ for δ in the range $\min(\delta\mu, 3\delta, 2-\delta) \;>\; 1$.

Proof. The proof is almost the same as the proof of the existence of γ_a^+. The modifications are as follows. Instead of (4.9) we first show that

$$\operatorname*{s\text{-}lim}_{t \to \infty} e^{iH_a t} \gamma_{a,t} e^{-iHt} (H+c)^{-2} \;=\; \operatorname*{s\text{-}lim}_{t \to \infty} (H_a + c)^{-1} e^{iH_a t} \gamma_{a,t} e^{-iHt} (H+c)^{-1}\,.$$

This follows from

$$\begin{aligned} &(\gamma_{a,t} - \partial_t g_{a,t})(H+c)^{-1} - (H_a+c)^{-1}(\gamma_{a,t} - \partial_t g_{a,t}) \\ &= (H_a+c)^{-1}\big([H, \gamma_{a,t} - \partial_t g_{a,t}] - I_a(\gamma_{a,t} - \partial_t g_{a,t})\big)(H+c)^{-1}\,. \end{aligned} \tag{5.2}$$

The extra term involving I_a gives no contribution in the limit $t \to \infty$ since by (3.27) $|I_a(x)| \leq \mathrm{const.}\, t^{-\delta\mu}$ on $\mathrm{supp}(g_{a,t})$. Therefore it suffices to prove convergence of

$$\varphi_t \;=\; (H_a + c)^{-1} e^{iH_a t} \widetilde{\gamma}_{a,t} e^{-iHt} (H + c)^{-1} \psi\,,$$

where $\widetilde{\gamma}_{a,t} = \gamma_{a,t} - 2\partial_t g_{a,t}$. Instead of (4.11) we then obtain

$$\partial_t \varphi_t \;=\; (H_a + c)^{-1} e^{iH_a t} (D_t \widetilde{\gamma}_{a,t} - i I_a \widetilde{\gamma}_{a,t}) e^{-iHt} (H + c)^{-1} \psi\,. \tag{5.3}$$

Here the term involving I_a gives an integrable contribution of order $t^{-\delta\mu}$ by (3.28). The rest of the proof goes through because the propagation estimate (3.20) also holds for the dynamics generated by H_a. □

Remark. Since the roles of H and H_a in the proof of Theorem 5.1 are interchangeable, we also have

$$(\omega_a^+)^* \;=\; \operatorname*{s-lim}_{t\to\infty} e^{iHt} \gamma_{a,t} e^{-iH_a t} \qquad \text{on } \; D(|p|) \tag{5.4}$$

Lemma 5.2. *If $I_a = O(|x|_a^{-\mu})$, $\mu > 1$, then any orbit ψ_t in the range of γ^+ is asymptotically clustering:*

$$\psi_t \underset{\|\,\|}{\longrightarrow} \sum_{a > \{0\}} e^{-iH_a t} \varphi_a \qquad (t \to \infty)\,. \tag{5.6}$$

Proof. Let $\psi = \gamma^+ \varphi$ ($\varphi \in \; D(|p|)$). By Theorem 4.1

$$\psi \;=\; \sum_{a > \{0\}} \gamma_a^+ \varphi \underset{\|\,\|}{\longrightarrow} \sum_{a > \{0\}} e^{iHt} \gamma_{a,t} e^{-iHt} \varphi\,,$$

and by Theorem 5.1

$$e^{-iHt}\psi \underset{\|\,\|}{\longrightarrow} \sum_{a > \{0\}} e^{-iH_a t} e^{iH_a t} \gamma_{a,t} e^{-iHt} \varphi \underset{\|\,\|}{\longrightarrow} \sum_{a > \{0\}} e^{-iH_a t} \omega_a^+ \varphi. \tag{5.7}$$

□

Lemma 5.2 together with (4.22) completes the proof of Theorem 2.1.

6. APPROACH TO THE LONG-RANGE CASE

We want to set up an inductive proof of asymptotic completeness for the dynamics U_t : $\psi \to \psi_t$ generated by

$$H_t \;=\; H + W_t(x)$$

for $1 \le t < \infty$ with the initial condition $U_1 = 1$. We assume that

$$\begin{aligned} \partial_x^k I_a(x) \;&=\; O(|x|_a^{-\mu-|k|}); \\ |\partial_{x,t}^k W_t(x)| \;&\le\; \text{const.}(1+|x|+t)^{-\mu-|k|}, \end{aligned} \qquad (0 \le |k| \le n) \tag{6.1}$$

where k is a multiindex and $\partial_{x,t}$ any derivative with respect to x or t. The conditions for μ and n will be given for each step. To begin with we only demand that $\mu > 0$ and $n = 1$. Since W_t is bounded it is elementary to construct U_t. $D(H) = D(H_t)$ is invariant under U_t, and since

$$\partial_t(U_t^{-1} H_t U_t) \;=\; U_t^{-1}(\partial_t W_t)U_t$$

is norm-integrable, the limits

$$H^+ \;:=\; \lim_{t\to\infty} U_t^{-1} H_t U_t = \; \lim U_t^{-1} H U_t$$

exist in norm sense on $D(H)$ and $H^+ = H + B$, B bounded. It follows that

$$\begin{aligned} (z - H^+)^{-1} \;&=\; \lim_{t\to\infty} U_t^{-1}(z-H)^{-1}U_t \\ (z - H)^{-1} \;&=\; \lim_{t\to\infty} U_t(z-H^+)^{-1}U_t^{-1} \end{aligned} \tag{6.2}$$

for $z \notin \sigma(H) = \sigma(H^+)$. Also $D(|p|)$ (the form domain of H) is invariant under U_t and

$$\langle\; p^2 \;\rangle_t \;\le\; \text{const.}\langle H + c\rangle_\psi, \tag{6.3}$$

Since $D_t x = p$ it still follows that $D(|x|) \cap D(|p|)$ is U_t–invariant. These are the general properties of the dynamics which we have used in the short-range case. It is now straightforward to generalize the results of Sections 3 and 4. The Heisenberg derivative D_t refers to the evolution U_t. The expression (3.4) for $\gamma_t = D_t g_t$ remains unchanged, while the r.h.s. of (3.5) receives the additional term $-\nabla g_t \cdot \nabla W_t$ which is bounded in norm by const. $t^{-\delta(\mu+1)}$. As a result the basic propagation estimate (3.21) remains valid if δ is in the range

$$\frac{1}{3} \;<\; \delta \;<\; 1\,; \qquad \delta\,(\mu+1) \;>\; 1. \tag{6.4}$$

Under this condition the existence of

$$\gamma^+ \;=\; \underset{t\to\infty}{s\text{-lim}}\,\gamma(t) \;=\; \underset{t\to\infty}{s\text{-lim}}\,U_t^{-1}\gamma_t U_t \qquad \text{on} \quad D(|p|)$$

(and similarly for γ_a^+) follows as before. We remark that in the first step of the proof (4.9) is replaced by

$$\underset{t\to\infty}{s\text{-lim}}\,U_t^{-1}\gamma_t U_t (H^+ + c)^{-2} \;=\; \underset{t\to\infty}{s\text{-lim}}\,(H^+ + c)^{-1} U_t^{-1}\gamma_t U_t (H^+ + c)^{-1}$$

using (6.2), which leads to

$$[\gamma^+, H^+] \;=\; 0 \tag{6.5}$$

instead of $[\gamma^+, H] = 0$ (and similarly for γ_a^+). All the other properties of γ^+ and γ_a^+ listed in Theorem 4.1 remain the same. In particular γ^+ is independent of the choice of δ in the range (6.4). We now describe the induction proof. For each channel $a > \{0\}$ we introduce a hierarchy of time evolutions which interpolate between U_t and the quasi-free evolution $U_{a,t}^\infty$ of the fragments. These evolutions have the following names and generators:

$$\begin{aligned}
U_t \;&:\; H_t \;=\; H \;+ W_t(x)\,;\\
\widetilde{U}_{a,t} \;&:\; \widetilde{H}_{a,t} \;=\; H_a + W_{a,t}(x)\,;\\
U_{a,t} \;&:\; H_{a,t} \;=\; H_a + W_{a,t}(p_a t + x^a)\,;\\
U_{a,t}^\infty \;&:\; H_{a,t}^\infty \;=\; H_a + W_{a,t}(p_a t)\,.
\end{aligned} \tag{6.6}$$

Here

$$W_{a,t}(x) \;=\; \big(I_a(x) + W_t(x)\big)\chi_{a,t}(x)\,, \tag{6.7}$$

where $\chi_{a,t}$ is a smoothed characteristic function of the set

$$\{x \mid |x| \geq t^\delta R^-;\; |x|_a \geq |x|^{1-\varepsilon}\}\,, \tag{6.8}$$

with $\varepsilon > 0$ arbitrary small. In particular

$$\chi_{a,t}(\xi t) \;=\; 1 \qquad \text{if } \xi \in a^* \tag{6.9}$$

and t sufficiently large. It also follows from (3.27) that

$$\chi_{a,t} \;=1 \qquad \text{on} \;\; \mathrm{supp}(g_{a,t}) \tag{6.10}$$

if t is large. To compute derivatives of $\chi_{a,t}$ with respect to t and x one can use an explicit form of $\chi_{a,t}$ like

$$\chi_{a,t}(x) \;=\; \theta(t^{-\delta}|x| - R^-) \prod_{b\cap a<a} \theta\left(|x^b|\,|x|^{\varepsilon-1} - 1\right) \tag{6.11}$$

where θ is a regularized step function. We note that

$$U_{a,t}^{\infty} \;=\; e^{-iH_a t - i\alpha_{a,t}(p_a)}; \qquad \alpha_{a,t}(p_a) \;=\; \int_1^t ds\, W_{a,s}(p_a s)\,.$$

It follows from (6.9) that on each fibre $p_a = \xi \in a^*$ this phase is equivalent to

$$\alpha_{a,t}(p_a) \;=\; \int_{t_0(p_a)}^t ds\big(I_a(p_a s) + W_s(p_a s)\big)\,, \tag{6.12}$$

by a gauge transformation (2.18). Our goal is to prove the following generalization of Theorem 2.2:

Theorem 6.1. *Suppose that (6.1) holds for some $\mu > \sqrt{3} - 1$ and $n = 2$. Then any $\psi \in \mathcal{H}$ is an outgoing scattering state for the dynamics U_t generated by H_t:*

$$U_t\psi \underset{\|\,\|}{\longrightarrow} \sum_a e^{-iH_a t - i\alpha_{a,t}(p_a)}\varphi_a \quad (t \to \infty) \tag{6.13}$$

for some $\varphi_a \in \mathcal{H}_a$. Here $\alpha_{a,t}(p_a)$ is given by (6.12) for $a > \{0\}$ and

$$\alpha_{\{0\},t} \;=\; \int_1^t ds\, W_s(0)\,. \tag{6.14}$$

Outline of the proof. The proof is given in three steps:

Step 1: Existence of the Deift–Simon wave operators

$$\omega_a^+ \;=\; \underset{t\to\infty}{s\text{-lim}}\, U_{a,t}^{-1}\gamma_{a,t}U_t \qquad \text{on} \;\; D(|p|). \tag{6.15}$$

This is proved in section 7. It follows as in Lemma 5.2 that any $\psi \in \mathrm{Ran}(\gamma^+)$ is asymptotically clustering: if $\psi = \gamma^+\varphi$ then

$$U_t\psi \underset{\|\,\|}{\longrightarrow} \sum_{a>\{0\}} U_{a,t}\varphi_a\,; \qquad \varphi_a = \omega_a^+\varphi\,. \tag{6.16}$$

Step 2: Induction step. We note that $H_{a,t}$ and $H_{a,t}^\infty$ commute with p_a. For each fiber $p_a = \xi \in a$ they reduce to operators acting on $L^2(a^\perp)$ given by

$$\begin{aligned} H_{a,t}(\xi) \;&=\; H^a + \frac{1}{2}\,\xi^2 + W_{a,t}(\xi\,t + x^a)\;; \\ H_{a,t}^\infty(\xi) \;&=\; H^a + \frac{1}{2}\,\xi^2 + W_{a,t}(\xi\,t) \end{aligned} \tag{6.17}$$

The Hamiltonian $H_{a,t}(\xi)$ has the same general form as H_t. Moreover it is not difficult to check that for any $\xi \in a^*$ the properties (6.1) are essentially inherited by the corresponding potential $W_{a,t}(\xi\,t + x^a)$. The only difference is that the exponents $(\mu + |k|)$ in (6.1) change into $(\mu+|k|)(1-\varepsilon)$, where ε is the parameter occurring in (6.8). Since ε is arbitrary small this difference is irrelevant and we ignore it. Now we invoke the induction hypothesis that asymptotic completeness in the form (6.13) holds for the dynamics $U_{a,t}(\xi)$ generated by $H_{a,t}(\xi)$ for each fiber $\xi \in a^*$. Integrating over the fibers gives for any $\varphi_a \in \mathcal{H}$:

$$U_{a,t}\varphi_a \underset{\|\,\|}{\longrightarrow} \sum_{b\geq a} e^{-iH_bt - i\alpha_{b,t}(p_b)}\varphi_{ab}; \quad (t\to\infty); \qquad \varphi_{ab} \in L^2(b)\otimes\mathcal{H}_B(H^b)\,. \tag{6.18}$$

Inserting this into (6.16) we see that any $\psi \in \mathrm{Ran}(\gamma^+)$ is an outgoing scattering state.

Step 3: The core of the proof is to show that (6.13) also holds for ψ in the kernel of γ^+. In section 8 we prove that $\gamma^+\psi = 0$ implies

$$U_t\psi \underset{\|\,\|}{\longrightarrow} e^{-iHt - i\alpha_{\{0\},t}}\varphi\,; \qquad \varphi \in \mathcal{H}_B(H)\,. \tag{6.19}$$

These three steps complete the proof of Theorem 6.2.

7. DEIFT-SIMON WAVE OPERATORS

Here we use the intermediate evolution $\widetilde{U}_{a,t}$ of (6.6) to factorize

$$\omega_a^+ \;=\; w_a^+ \cdot \widetilde{\omega}_a^+ \,;$$

$$w_a^+ \;=\; \underset{t\to\infty}{s\text{-lim}}\, U_{a,t}^{-1}\widetilde{U}_{a,t}; \qquad \widetilde{\omega}_a^+ \;=\; \underset{t\to\infty}{s\text{-lim}}\, \widetilde{U}_{a,t}^{-1}\gamma_{a,t}U_t. \tag{7.1}$$

Lemma 7.1. *If (6.1) holds for $\mu > 0$ and $n = 1$ then $\widetilde{\omega}_a^+$ exists on $D(|p|)$, provided that δ is taken in the range (6.4).*

Proof. The proof is analogous to the proof of Theorem 5.1. We start from the equivalence

$$\underset{t\to\infty}{s\text{-lim}}\, \widetilde{U}_{a,t}^{-1}\gamma_{a,t}U_t(H^+ + c)^{-2} = \underset{t\to\infty}{s\text{-lim}}\, (\widetilde{H}_a^+ + 1)^{-1}\widetilde{U}_{a,t}^{-1}\gamma_{a,t}U_t(H^+ + c)^{-1} \;.$$

This follows from (6.2) and from an identity similar to (5.2), where the term $I_a(\gamma_{a,t} - \partial_t g_{at})$ is now replaced by

$$(H_t - \widetilde{H}_{a,t})(\gamma_{a,t} - \partial_t g_{a,t}) \;=\; (I_a + W_t)(1 - \chi_{a,t})(\gamma_{a,t} - \partial_t g_{a,t})\,. \tag{7.2}$$

This term vanishes exactly for t sufficiently large by (6.10). Then we have to prove convergence of

$$\varphi_t \;=\; (\widetilde{H}_a^+ + 1)\widetilde{U}_{a,t}^{-1}\widetilde{\gamma}_{a,t}U_t(H^+ + c)^{-1}\,,$$

where $\widetilde{\gamma}_{a,t} = \gamma_{a,t} - 2\partial_t\, g_{a,t}$. Instead of (5.3) we obtain

$$\partial_t\varphi_t \;=\; (\widetilde{H}_a^+ + c)^{-1}\widetilde{U}_{a,t}^{-1}(D_t\widetilde{\gamma}_{a,t})U_t(H^+ + c)^{-1}$$

since the term $(H_t - \widetilde{H}_{a,t})\widetilde{\gamma}_{a,t}$ vanishes again by (6.10). Strong integrability of $\partial_t\varphi_t$ follows as before from the propagation estimate (3.20), which also holds for the evolution $\widetilde{U}_{a,t}$. □

Lemma 7.2. *If (6.1) holds for $\mu > 1/2$ and $n = 2$ then w_a^+ exists on $\mathcal{H}$ provided that δ is taken in the range*

$$\frac{1}{3} < \delta < 1; \quad \delta(\mu+1) > \frac{3}{2}; \quad \delta(\mu+2) > 2\,. \tag{7.3}$$

Proof. Using Cook's argument we want to show that

$$\partial_t U_{a,t}^{-1} \widetilde{U}_{a,t} \; = \; -iU_{a,t}^{-1}[W_{a,t}(x) - W_{a,t}(p_a t + x^a)]\widetilde{U}_{a,t}\psi$$

is integrable for a dense set of ψ's. The middle term can be expressed as

$$\begin{aligned}[\ldots] \; = \; & \int_0^1 ds\, \nabla_a W_{a,t}\big(sx_a + (1-s)p_a t + x^a\big) \cdot (x_a - p_a t) \\ & + \frac{it}{2} \int_0^1 ds\, \Delta_a W_{a,t}\big(sx_a + (1-s)p_a t + x^a\big)\,. \end{aligned} \tag{7.4}$$

(This identity comes from evaluating

$$f(x) - f(pt) = \int_0^1 ds\, \frac{d}{ds} f(pt + s(x - pt)).$$

Representing $f(x)$ by a Fourier integral, say for $f \in \mathcal{S}(R^n)$, it suffices to consider the case $f(x) = \exp(ik\cdot x)$. Then

$$e^{ik\cdot(pt+s(x-pt))} = e^{itk\cdot p}\; e^{isk\cdot(x-pt)}\; e^{-\frac{i}{2}stk^2}$$

by the Campbell–Hausdorff formula. Now the s–derivative is computed and inserted into the Fourier integral. This proves (7.4) for $W_t(\cdot) \in \mathcal{S}(R^n)$, and our bounds for ∇W_t and ΔW_t allow it to extend the result by a limiting argument). From (6.7) and (6.11) it follows that

$$\|\Delta_a W_{a,t}\| = \sup_x \; |\Delta_a W_{a,t}(x)| \leq (1+t)^{-\delta(\mu+2)(1-\varepsilon)}.$$

Since ε is arbitrary small we drop the factor $(1-\varepsilon)$. The second term in (7.4) is therefore norm-bounded by const.$\,t^{1-\delta(\mu+2)}$, which is integrable since $\delta(\mu+2) > 2$. Similarly, the contribution of the first term is bounded by

$$\text{const.}\, t^{-\delta(\mu+1)} \langle\, (x_a - p_a t)^2 \,\rangle_t^{1/2} \tag{7.5}$$

where $\langle \cdots \rangle_t$ is taken for the evolution $\psi_t = \widetilde{U}_{a,t}\psi$. Let $\widetilde{D}_t$ be the corresponding Heisenberg derivative. Then

$$\begin{aligned}\widetilde{D}_t(x_a - p_a t) \; &= \; i[\widetilde{H}_{a,t}, x_a - p_a t] - p_a \; = \; i[W_{a,t}(x), x_a - p_a t] \\ &= \; t\nabla_a W_{a,t}(x) \; = O(t^{1-\delta(\mu+1)})\,.\end{aligned}$$

uniformly in x. Therefore

$$\begin{aligned}\partial_t\langle\, (x_a - p_a t)^2 \,\rangle_t \; &\le \; \text{const.}\, t^{1-\delta(\mu+1)} \langle\, (x_a - p_a t)^2 \,\rangle_t^{1/2} \quad , \text{ or} \\ \partial_t\langle (x_a - p_a t)^2\rangle^{1/2} \; &\le \; \text{const.}\, t^{1-\delta(\mu+1)}\,.\end{aligned}$$

Taking $\psi \in D(|x|) \cap D(|p|)$ this gives

$$\langle\, (x_a - p_a t)^2 \,\rangle_t^{1/2} \; \le \; \text{const.}\, t^{2-\delta(\mu+1)}\,.$$

Together with (7.5) we see that the contribution of the first term in (7.4) is integrable if $2\delta(\mu + 1) > 3$. □

We remark that this proof is the only instance where we use the *second* derivatives of $I_a(x)$ and $W_t(x)$ with respect to x. As a result we have:

Theorem 7.3. *If (6.1) holds for $\mu > 1/2$ and $n = 2$ then the Deift-Simon wave operators*

$$\omega_a^+ \; = \; \operatorname*{s\text{-}lim}_{t\to\infty} U_{a,t}^{-1}\gamma_{a,t}U_t$$

exist on $D(|p|)$ provided that δ is taken in the range

$$\frac{1}{3} < \delta < 1; \quad \delta(\mu+1) > \frac{3}{2}; \quad \delta(\mu+2) > 2\,. \tag{7.6}$$

Remark. This Theorem and its proof using the factorization (7.1) are due to Dereziński and Gérard [DerGer1].

Corollary 7.3. *The adjoints of ω_a^+ exist as strong limits*

$$(\omega_a^+)^* \; = \; \operatorname*{s\text{-}lim}_{t\to\infty} U_t^{-1}\gamma_{a,t}\,U_{a,t} \qquad \text{on} \;\; D(|p|). \tag{7.7}$$

Proof. The roles of U_t, $\widetilde{U}_{a,t}$ in the proof of Lemma 7.1 and of $U_{a,t}$, $\widetilde{U}_{a,t}$ in the proof of Lemma 7.2 are interchangeable. □

8. PROPAGATION ON KER(γ^+)

Theorem 8.1. *Let $\gamma^+\psi = 0$ and suppose that (6.1) holds for $\mu > \sqrt{3} - 1$ and $n = 1$. Then*

$$U_t\psi \underset{\|\,\|}{\longrightarrow} e^{-iHt - i\int_1^t ds\, W_s(0)}\varphi \quad (t \to \infty); \qquad \varphi \in \mathcal{H}_B(H)\,. \tag{8.1}$$

Remarks. The scaling parameter δ does not appear in this theorem. However, we will need the propagation estimate (3.20) and the representation of γ^+ as the strong limit (4.4), i.e. some choice of δ in the range

$$\frac{1}{3} < \delta < 1\,; \qquad \delta(\mu + 1) > 1\,, \tag{8.2}$$

in which γ^+ is independent of δ (Theorem 4.1). For the proof we also need the additional conditions

$$\delta < \mu\,; \qquad \delta(\mu + 2) > 2\,. \tag{8.3}$$

(8.2) and (8.3) can both be satisfied if $\mu(\mu + 2) > 2$, i.e if $\mu > \sqrt{3} - 1$. The proof of Theorem 8.1 is given in 3 steps (Lemmas 8.2–8.4 below), where we use the notation and the results of Appendix C. We also recall

$$U^{\infty}_{\{0\},t} \;:=\; e^{-iHt - i\int_1^t ds\, W_s(0)}\,. \tag{8.4}$$

Lemma 8.2. *Let $\delta < \delta' < \mu$ and $\theta > 0$. Then*

$$\omega^+_{\{0\}} \;=\; \underset{t\to\infty}{s\text{-}\lim}\, (U^{\infty}_{\{0\},t})^{-1}\chi(t^{-\delta'}g_t \le \theta)U_t \tag{8.5}$$

exists on $\mathcal{H}$.

Lemma 8.3. *If $\gamma^+\psi = 0$ then*

$$\omega^+_{\{0\}}\psi \;=\; \lim_{t\to\infty} (U^{\infty}_{\{0\},t})^{-1}U_t\psi\,. \tag{8.6}$$

Lemma 8.4. *If $\gamma^+\psi = 0$ and*

$$U_t\psi \underset{\|\,\|}{\longrightarrow} e^{-iHt-i\alpha(t)}\varphi \quad (t \to \infty) \tag{8.7}$$

for some real phase $\alpha(t)$, then $\varphi \in \mathcal{H}_B(H)$.

Proof of Lemma 8.2. Since

$$\|[(H+c)^{-1}, \chi(t^{-\delta'} g_t \le \theta)]\| \;=\; O(t^{-\delta'})$$

it suffices to prove strong convergence of

$$\phi_t \;=\; (U^\infty_{\{0\},t})^{-1}(H+c)^{-1}\chi(t^{-\delta'} g_t \le \theta)(H+c)^{-1}U_t\,.$$

Proceeding as in the proof of Theorem 4.1 we estimate

$$\begin{aligned}\partial_t\phi_t \;&=\; (U^\infty_{\{0\},t})^{-1}(H+c)^{-1}(D_t\chi)(H+c)^{-1}U_t \\ &\quad + (U^\infty_{\{0\},t})^{-1}(H+c)^{-1}[W_t(0) - W_t(x)]\chi(H+c)^{-1}U_t,\end{aligned}$$

where D_t is the Heisenberg derivative for U_t. The first term is strongly integrable by Theorem C.2 and by the argument given in (4.12).The same is true for the second term since $|x| \le$ const.$t^{\delta'}$ on supp$(\chi(t^{-\delta'} g_t \le \theta)$. Using (6.1) we thus obtain

$$\|(W_t(0) - W_t(x))\chi(t^{-\delta'} g_t \le \theta)\| = O(t^{\delta'-\mu-1}),$$

which is integrable since $\delta' < \mu$. □

Proof of Lemma 8.3. Since $[\gamma^+, H^+] = 0$ it suffices to prove (8.6) for $\psi \in D(H)$. By Lemma 8.2 we need only show that for $\psi_t = U_t\psi$

$$\lim_{t\to\infty} \chi(t^{-\delta'} g_t \ge \theta)\psi_t \;=\; 0$$

for $\theta > 0$ or, by (C.5), that

$$\lim_{t\to\infty} \chi(t^{1-\delta'}\Gamma_t \ge \theta_1)\psi_t \;=\; 0 \tag{8.8}$$

for $\theta_1 > 0$. Since $\|\partial_t g_t\| \to 0$, $\gamma^+\psi = 0$ implies that $\Gamma_t\psi_t \to 0$ for $t \to \infty$, and therefore

$$\lim_{s\to\infty} \chi(b\Gamma_s \geq \theta_1)\psi_s = 0$$

for any $b > 0$. Using this and Lemma C.3 we can estimate

$$\begin{aligned}\langle\chi(b\Gamma_s \geq \theta_1)\rangle_s &= -\int_s^\infty dt\ \langle D_t\,\chi(b\Gamma_s \geq \theta_1)\rangle_t \\ &\leq \text{const.}(b^3 s^{1-3\delta} + bs^{1-\delta(\mu+1)})\|\psi\|_H^2\,.\end{aligned}$$

Setting now $s = t$, $b = t^{1-\delta'}$ we obtain

$$\langle\chi(t^{1-\delta'}\Gamma_t \geq \theta_1)\rangle_t \;=\; O(t^{4-6\delta}) + O(t^{2-\delta(\mu+2)})$$

which vanishes as $t \to \infty$. Replacing χ by χ^2 we arrive at (8.8). □

Proof of Lemma 8.4. Again we can assume that $\psi \in D(H^+)$. Then (8.6) and (6.2) imply $\varphi \in D(H)$ and

$$0 \;=\; \lim_{t\to\infty}(\psi, U_t^{-1}\gamma_t U_t\psi) \;=\; \lim_{t\to\infty}(\varphi, e^{iHt}\gamma_t e^{-iHt}\varphi) \;=\; (\varphi, \gamma_H^+\varphi)\,,$$

where γ_H^+ is the asymptotic observable γ^+ for the time evolution generated by H. Since $\gamma_H^+ \geq 0$ this implies $\gamma_H^+\varphi = 0$ and therefore $\varphi \in \mathcal{H}_B(H)$ by (4.22). □

9. LONG–RANGE WAVE OPERATORS

In this section we prove the existence of the wave operators in the long–range case for the dynamics U_t generated by H_t.

Theorem 9.1. *Suppose that (6.1) holds for some $\mu > \sqrt{3} - 1$ and $n = 2$. Then the wave operators*

$$\Omega_a^+ \;=\; s\text{-}\lim_{t\to\infty}\; U_t^{-1}\, U_{a,t}^\infty \tag{9.1}$$

exist on $\mathcal{H}_a$ for all $a \in L$ and have mutually orthogonal ranges

$$\mathcal{H}_a^+ \;\perp\; \mathcal{H}_b^+ \qquad (a \neq b)\,. \tag{9.2}$$

The proof of this theorem uses the results of sections 7 and 8. The first step is to prove the special case $a = \{0\}$:

Lemma 9.2. *Under the hypothesis of Theorem 9.1. the wave operator*

$$\Omega^{+}_{\{0\}} \;=\; s\text{-}\lim_{t\to\infty}\; U_t^{-1}\, U^{\infty}_{\{0\},t} \tag{9.3}$$

exists on $\mathcal{H}_B(H)$.

Proof. Let ψ be an eigenvector of H. Since the time evolution $\psi_t = U^{\infty}_{\{0\},t}\,\psi$ affects only the phase of ψ it follows directly that

$$\lim_{t\to\infty}\; \|\chi(t^{-\delta'} g_t \geq \theta)\,\psi_t\| \;=\; 0$$

for $\delta' > \delta$. Therefore it suffices to establish strong convergence of

$$U_t^{-1}\,\chi(t^{-\delta'} g_t \leq \theta)\, U^{\infty}_{\{0\},t}\;.$$

This is proven like Lemma 8.2, with the roles of the two propagators interchanged. □

Our goal is to prove convergence of (9.1) for $a > \{0\}$ on the states of the form

$$\psi(x) \;=\; \varphi(x_a)\, u(x^a);\quad \widehat{\varphi}\in C_0^{\infty}(a^*);\quad H^a u = \lambda u, \tag{9.4}$$

where $\widehat{\varphi}$ is the Fourier transform of φ. These states span a dense set in $\mathcal{H}_a$.

Lemma 9.3. *Under the hypothesis of Theorem 9.1 the limits*

$$\lim_{t\to\infty}\; U_t^{-1}\,\gamma_{a,t}\, U^{\infty}_{a,t}\,\psi \tag{9.5}$$

exist for $a > \{0\}$ and any ψ of the form (9.4).

Proof. We factorize

$$U_t^{-1}\,\gamma_{a,t}\,U^{\infty}_{a,t}\,\psi \;=\; (U_t^{-1}\,\gamma_{a,t}\,U_{a,t})(U_{a,t}^{-1}\,U^{\infty}_{a,t})\,\psi\;.$$

The first factor converges strongly on the form domain of H by Corollary (7.3). The second factor commutes with p_a, so it suffices to prove convergence of $U_{a,t}^{-1}\,U^{\infty}_{a,t}\,\psi$ in $\mathcal{H}^a$ for each fiber $p_a = \xi \in a^*$. Recalling the generators (6.17) this follows from Lemma 9.2., applied to $H^a + W_{a,t}(\xi t + x^a)$ in place of H_t. □

Lemma 9.4. *Suppose that (6.1) holds for some $\mu > 0$ and $n = 2$. Then, for $a > \{0\}$ and any fixed ψ of the form (9.4), we can choose the Yafaev function g such that*

$$\lim_{t\to\infty} (U_{a,t}^{\infty})^{-1} \gamma_{a,t} U_{a,t}^{\infty} \psi \;=\; \sigma_a \, |p_a| \, \psi, \qquad (\sigma_a > 0). \tag{9.6}$$

As a preparation for the proof we discuss the asymptotic form of the quasi–free evolution in $L^2(R^n)$:

$$\varphi_t \;=\; e^{-\frac{i}{2}tp^2} \varphi_t^0; \qquad \varphi_t^0 \;=\; e^{-i\alpha_t(p)} \varphi$$

for $\widehat{\varphi} \in C_0^\infty(R^n \setminus \{0\})$. Here

$$\alpha_t(p) \;=\; \int_1^t ds\, W_s(ps),$$

and $W_t(x)$ is assumed to satisfy (6.1) with $\mu > 0$ and $n = 2$. Then

$$\varphi_t(x) \;=\; (2\pi i t)^{n/2} \exp(\frac{ix^2}{2t}) \int dy \exp(-\frac{ix \cdot y}{t}) \exp(\frac{iy^2}{2t})\, \varphi_t^0(y).$$

The lowest order Taylor expansion of the last exponential leads to

$$\begin{aligned} \varphi_t(x) \;&=\; \widetilde{\varphi}_t(x) \;+\; R_t(x); \quad \widetilde{\varphi}_t(x) \;=\; (it)^{n/2} \exp(\frac{ix^2}{2t})\, \widehat{\varphi_t^0}\left(\frac{x}{t}\right); \\ \|R_t(\cdot)\|_2 \;&\le\; \frac{1}{t}\, \|\Delta\left(\exp(-i\alpha_t(\cdot))\, \widehat{\varphi}_0(\cdot)\right)\|_2 \;=\; O(t^{-\mu}). \end{aligned} \tag{9.7}$$

$\widetilde{\varphi}_t$ is the leading term for $t \to \infty$. The bound for R_t is obtained by estimating $\nabla\alpha_t(\cdot)$ and $\Delta\alpha_t(\cdot)$ using (6.1). As a result we have

$$\lim_{t\to\infty} \|\varphi_t - \widetilde{\varphi}_t\| \;=\; 0 \quad \text{and} \quad \lim_{t\to\infty} \|p_k\varphi_t - \left(\frac{x_k}{t}\right) \widetilde{\varphi}_t\| \;=\; 0\,. \tag{9.8}$$

The second limit follows from the first if φ is replaced by $p_k\varphi$.

Proof of Lemma 9.4. Given ψ of the form (9.4) we can choose the Yafaev function g such that for some $\varepsilon > 0$

$$g_a(x) \;=\; \sigma_a |x_a| \quad \text{if} \quad x \in \operatorname{supp}(\widehat{\varphi}) \quad \text{and} \quad |x^a| \le \varepsilon$$

(cf. Lemma A.3). Then

$$g_{a,t}(x) \;=\; \sigma_a |x_a| \quad \text{if} \quad \frac{x}{t} \in \operatorname{supp}(\widehat{\varphi}) \quad \text{and} \quad |x^a| \leq \varepsilon t$$

for $t > 1$. Since

$$\gamma_{a,t} \;=\; \nabla g_{a,t} \cdot p \;+\; O(t^{-\delta})$$

we have

$$\gamma_{a,t}\, U_{a,t}^{\infty}\, \psi \underset{\|\,\|}{\longrightarrow} \nabla g_{a,t} \cdot \big(p_a \varphi_t \otimes e^{-i\lambda t} u\big) + \nabla g_{a,t} \cdot \big(\varphi_t \otimes e^{-i\lambda t} p^a u\big),$$

where φ_t is the quasi–free evolution of φ in $L^2(a)$. Using (9.8) we obtain

$$\gamma_{a,t}\, U_{a,t}^{\infty}\, \psi \underset{\|\,\|}{\longrightarrow} \nabla g_{a,t} \cdot \big(\frac{x_a}{t} \widetilde{\varphi}_t \otimes e^{-i\lambda t} u\big) + \nabla g_{a,t} \cdot \big(\widetilde{\varphi}_t \otimes e^{-i\lambda t} p^a u\big). \tag{9.9}$$

The part of this wave function in the region $|x^a| > \varepsilon t$ vanishes in norm as $t \to \infty$ since u and $p^a u$ are in $L^2(a^{\perp})$. In the complementary region we have $\nabla g_{a,t} = \sigma_a x_a |x_a|^{-1} \in a$, so that the last term of (9.9) gives no contribution. Therefore

$$\gamma_{a,t}\, U_{a,t}^{\infty}\, \psi \underset{\|\,\|}{\longrightarrow} \sigma_a \frac{|x_a|}{t} \big(\widetilde{\varphi}_t \otimes e^{-i\lambda t} u\big) \underset{\|\,\|}{\longrightarrow} \sigma_a \, |p_a|\, U_{a,t}^{\infty}\, \psi. \qquad \square$$

Proof of Theorem 9.1. By (9.5) and (9.6)

$$\lim_{t\to\infty} \; U_t^{-1} \gamma_{a,t}\, U_{a,t}^{\infty}\, \psi \;=\; \lim_{t\to\infty} \; U_t^{-1}\, U_{a,t}^{\infty}\, \sigma_a |p_a| \psi \;=\; \Omega_a^{+}\, \sigma_a\, |p_a|\, \psi$$

exists. Since $\sigma_a\, |p_a|$ maps the class (9.4) onto itself, $\Omega_a^{+}\psi$ exists for all ψ in this class. (9.2) follows from

$$\lim_{t\to\infty} \, (U_{a,t}^{\infty}\, \psi_a \, , \, U_{b,t}^{\infty}\, \psi_b) \;=\; 0$$

for $a \neq b$ and $\psi_a, \; \psi_b$ of the form (9.4). This is readily obtained by using the asymptotic form (9.7). $\square$

A. THE YAFAEV CONSTRUCTION

In this appendix we describe the analytic construction of $g(x)$ as outlined in section 3. For $a > \{0\}$ and σ given in accordance with (3.22) we define the cones

$$\begin{aligned} C_a(\sigma) &= \{x \mid \sigma_a |x_a| > \sigma_b |x_b| \quad \forall\, b > a\} \ ; \\ U_a(\sigma) &= \{x \mid \sigma_a |x_a| > \sigma_X |x|\} \ ; \\ V_a(\sigma) &= \{x \mid \sigma_a |x_a| > \sigma_b |x| \quad \forall\, b > a\} \ . \end{aligned}$$

Evidently $V_a(\sigma) \subset C_a(\sigma) \subset U_a(\sigma)$ and

$$x \in U_a \Leftrightarrow (x^a)^2 < \left(1 - \frac{\sigma_X^2}{\sigma_a^2}\right) x^2; \quad x \in V_a \Leftrightarrow (x^a)^2 < \left(1 - \frac{\sigma_b^2}{\sigma_a^2}\right) x^2 \ \ \forall b > a.$$

We note that $V_a(\sigma)$ and hence $C_a(\sigma)$ contains the cone

$$(x^a)^2 < x^2 \cdot \min_{b>a} \left(1 - \frac{\sigma_b^a}{\sigma_a^2}\right) . \tag{A.1}$$

Lemma A.1. *There exists a choice of σ_a, $a > \{0\}$ such that for $a \cap b < a, b$*

$$U_a(\sigma) \cap U_b(\sigma) \subset V_{a\cap b}(\sigma) .$$

Proof. Let $0 < \varepsilon < 1$ and $|a| = \dim(a)$. We define σ_a by

$$1 - \frac{1}{\sigma_a^2} = \varepsilon^{2|a|} . \tag{A.2}$$

Then, for $b > a$,

$$\varepsilon^{2|a|} > \left(1 - \frac{\sigma_b^2}{\sigma_a^2}\right) = \frac{\varepsilon^{2|a|} - \varepsilon^{2|b|}}{1 - \varepsilon^{2|b|}} > \varepsilon^{2|a|}(1 - \varepsilon^2)$$

since $|b| \geq |a| + 1$. Now we use that

$$|x^{a\cap b}| \leq M \cdot \max(|x^a|, |x^b|)$$

for all x, a, b, where M is a constant depending only on the lattice L (Both sides are seminorms on X, and $|x^a| = |x^b| = 0$ implies $x \in a \cap b$, i.e. $|x^{a\cap b}| = 0$). Let $a \cap b = c < a, b$ and $x \in U_a \cap U_b$. Then

$$|x^c|^2 \;\le\; M^2 \cdot \max\left(\varepsilon^{2|a|}, \varepsilon^{2|b|}\right) x^2 \;\le\; M^2 \varepsilon^{2(|c|+1)} x^2 \,.$$

It follows that $x \in V_c(\sigma)$ if $M^2 \varepsilon^{2(|c|+1)} \le \varepsilon^{2|c|}(1-\varepsilon^2)$, i.e. if $\varepsilon^2 \;\le\; (1+M^2)^{-1}$. □

Lemma A.1 and (A.1) show that the family of cones $C_a(\sigma)$ has all the properties required by the condition (Y.2) of section 3. In particular it follows from (A.1) and Lemma 3.1 that

$$|x|_a^2 \;\ge\; x^2 \cdot \min_{b>a} \left(1 - \frac{\sigma_b^2}{\sigma_a^2}\right) \qquad \text{on } C_a^*(\sigma)\,.$$

Now we fix σ as follows. For $a > \{0\}$ we set $\sigma_a^2 \;=\; (1-\varepsilon^{2|a|})^{-1}$ in accordance with (A.2), with ε in the range

$$0 \;<\; \varepsilon^2 \;\le\; (2+M^2)^{-1}\,. \tag{A.3}$$

Then we fix $\sigma_{\{0\}}$ (arbitrary large) in accordance with (3.23).

Lemma A.2. *Let $a > \{0\}$ and $m_a(x) \;:=\; \max(\sigma_{\{0\}}, \sigma_a|x_a|) \;=\; m_a(x_a)$. Then*

(i) *If $x \in C_a^*(\sigma)$ then $\widehat{g}(x,\sigma) \;=\; m_a(x_a)$.*

(ii) *$\widehat{g}_a(x,\sigma)$ has support in $\overline{C_a^*(\sigma)}$, where $\widehat{g}_a(x,\sigma) \;=\; \sigma_a(x_a)\theta(\sigma_a|x_a| - \sigma_{\{0\}})$.*

(iii) *If $x \in C_a(\sigma)$ then $\widehat{g}(x,\sigma) = \max_{b\le a}\big(m_b(x_b)\big) = \widehat{g}(x_a,\sigma)$ and*

$$\widehat{g}_{\{0\}}(x,\sigma) = \sigma_{\{0\}}\theta\big(\sigma_{\{0\}} - \widehat{g}(x_a,\sigma)\big) = \widehat{g}_{\{0\}}(x_a,\sigma)\ .$$

(iv) *If $x \in C_a(\sigma)$ and $b > \{0\}$ then $\widehat{g}_b(x,\sigma) = 0$ unless $b \le a$. In that case*

$\widehat{g}_b(x,\sigma) = m_b(x_b)[m_b(x_b) - \widehat{g}(x_a,\sigma)]$, in particular $\widehat{g}_b(x,\sigma) \;=\; \widehat{g}_b(x_a,\sigma)$.

Proof. (i) Let $x \in C_a^*(\sigma)$ and $\widehat{g}(x,\sigma) > \sigma_{\{0\}}$ (else the statement is trivial). It suffices to restrict x to the set where the maximal piece of $\widehat{g}$ is unique, i.e.

$$\widehat{g}(x,\sigma) \;=\; \sigma_b|x_b| \;>\; \sigma_c|x_c| \tag{A.4}$$

for some $b > 0$ and all $c \neq b$, which implies $x \in C_b(\sigma)$. We have to show that $b = a$. $b < a$ is excluded since $x \in C^*_a(\sigma)$. $b \cap a < a, b$ is equally excluded since then $x \in C_{a\cap b}(\sigma)$. Finally $b > a$ is excluded since (A.4) states that $\sigma_b|x_b| > \sigma_a|x_a|$ which contradicts $x \in C_a(\sigma)$.
(ii) follows from (i) since the sets $C^*_a(\sigma)$ form a disjoint covering of X, and since the decomposition of $\widehat{g}$ into maximal pieces is unique. (iii) follows from (i) since

$$C_a(\sigma) \ = \ \bigcup_{b\leq a} C^*_b(\sigma)$$

and since $x_b = (x_a)_b$ for $b \leq a$. (iv) follows from (iii) by reading off the maximal pieces of $\widehat{g}$ on $C_a(\sigma)$. □

To perform the regularisation (3.24) explicitly we treat the parameters σ_a as variables, restricted to disjoint intervals

$$\sigma^-_a \ < \ \sigma_a \ < \ \sigma^+_a\,, \tag{A.5}$$

which requires $\sigma^+_a < \sigma^-_b$ for $b < a$. A possible choice is

$$(\sigma^-_a)^2 \ = \ (1 - \varepsilon^{2|a|})^{-1}\,; \qquad (\sigma^+_a)^2 \ = \ (1 - 2\varepsilon^{2|a|})^{-1}$$

for $a > \{0\}$, with ε in the range (A.3). $\sigma^{\pm}_{\{0\}}$ is fixed with $\sigma^+_{\{0\}} > \sigma^-_{\{0\}} > \sigma^+_a \ \forall a > \{0\}$. For $a > \{0\}$ we define

$$C^{\pm}_a \ = \ \{x \mid \sigma^{\pm}_a|x_a| > \sigma^{\mp}_b|x_b| \ \forall b > a\} \tag{A.6}$$

so that

$$C^-_a \ \subset \ C_a(\sigma) \ \subset \ C^+_a \tag{A.7}$$

for all σ allowed by (A.5). As in the proof of Lemma A.1 it follows from (A.3) that

$$C^+_a \cap C^+_b \ \subset \ C^-_{a\cap b} \qquad \text{if } a \cap b < a, b\,, \tag{A.8}$$

so that the functions $\widehat{g}(x, \sigma)$ have the properties listed in Lemma A.2 for all allowed σ.

Now we pick arbitrary weight functions $0 \le \delta_a \in C_0^\infty(\sigma_a^-, \sigma_a^+)$, normalized to $\int ds\, \delta_a(s) = 1$, and we set $j_a(s) = \int_{-\infty}^s dt\, \delta_a(t)$. The regularisation of $\widehat{g}(x,\sigma)$ is then defined by

$$g(x) = \int \widehat{g}(x,\sigma) \prod_{c\in L} \left(\delta_c(\sigma_c) d\sigma_c\right), \tag{A.9}$$

and similarly for $g_a(x)$. For $a > \{0\}$ we insert the explicit form

$$\widehat{g}_a(x,\sigma) = \sigma_a |x_a| \theta(\sigma_a |x_a| - \sigma_{\{0\}}) \prod_{\{0\}>b\neq a} \theta(\sigma_a |x_a| - \sigma_b |x_b|),$$

which gives

$$g_a(x) = |x_a| \int ds\, s\delta_a(s) j_0(s|x_a|) \prod_{\{0\}<b\neq a} j_b\left(\frac{s|x_a|}{|x_b|}\right)$$

and similarly for $g_{\{0\}}(x)$. These formulas only serve to exhibit the smoothness of the functions g and g_a. All the other relevant properties of g and g_a follow directly from Lemma A.2 via (A.14) and (A.16). The result is:

Lemma A.3. *The function g constructed above is a Yafaev function with respect to the cones C_a^- (A.6). Moreover, g has a decomposition (3.25) into smooth functions g_a with the following properties. There exist constants $0 < \bar\sigma_a$ and $0 < R^- < R^+$ such that*

(i) *For $a = \{0\}$:*

$$\mathrm{supp}(g_{\{0\}}) \subset \{|x| < R^+\};$$

$$g_{\{0\}}(x) = g(0) = \bar\sigma_{\{0\}} \text{ if } |x| < R^-;$$

$$g_{\{0\}}(x) = g_{\{0\}}(x_b) \text{ on } C_b^- \quad \forall b > \{0\}.$$

(ii) *For $a > \{0\}$:*

$$\mathrm{supp}(g_a) \subset \{|x| > R^-\} \cap \left(C_a^+ \setminus \textstyle\bigcup_{b<a} C_b^-\right);$$

$$g_a(x) = g(x) = \bar\sigma_a |x_a| \text{ on } C_a^- \setminus \textstyle\bigcup_{b<a} C_b^+;$$

$g_a(x)$ is homogeneous of degree 1 for $|x| > R^+$;

$$g_a(x) \;=\; g_a(x_b) \text{ on } C_b^- \quad \forall b > \{0\}.$$

Corollary A.3. *There exists $\lambda > 0$ such that:*

(i) *If $a > \{0\}$ and $x \in \mathrm{supp}(g_a)$, then $|x|_a \;\geq\; \lambda|x| \;\geq\; \lambda R^-$.*

(ii) *If $a \geq \{0\}$, $b > \{0\}$ and $x \in \mathrm{supp}(\nabla g_a) \cap (C_b^-)^*$, then*

$$\nabla g_a(x) \in b \text{ and } |x|_b \geq \lambda|x| \geq \lambda R^- .$$

Proof. (i) follows from

$$C_b^- \cap \Big(C_a^+ \setminus \bigcup_{c<a} C_c^-\Big) \;=\; \phi \text{ if } b \cap a < a\,,$$

which is proved like (3.13) using (A.8). (ii) follows directly from the fact that $g_a(x) = g_a(x_b)$ on C_b^-. □

Lemma A.4. *Suppose that f is a function on X which has all the properties of a Yafaev function except convexity: f is smooth; $f(x) = f(x_a)$ near a (in particular $f(x) = 0$ for $|x| < R_1$); and $f(\lambda x) = \lambda f(x)$ for $|x| > R_2$ ($\lambda > 1$). Then there exists a Yafaev function $\widetilde{g}$ such that the Hessians of f and $\widetilde{g}$ satisfy*

$$\pm f''(x) \;\leq\; \widetilde{g}''(x) \qquad \forall x\,. \tag{A.10}$$

Proof. For any fixed $y \in X$, $y \neq 0$ we first construct a *local bound,* i.e. a Yafaev function $\widetilde{g}$ such that (A.10) holds for x near y. Since $y \in a^*$ for some $a > \{0\}$ there exists a Yafaev function g with $g(x) = \sigma|x_a|$ near y so that

$$g''(x) \;=\; \frac{\sigma}{|x_a|}\,\pi_a(x)\,,$$

where $\pi_a(x)$ is the projection of X into a given by

$$\xi \longrightarrow \xi_a - \frac{1}{|x_a|^2}\,(x_a \cdot \xi)x_a\,,$$

which has rank $\dim(a) - 1$. Since $f(x) = f(x_a)$ near $y \in a$, $f''(x)$ also maps X into a. However, $f''(x)$ may have full rank $= \dim(a)$ in the shell $R_1 < |x| < R_2$ where f is not homogeneous. For this reason we first replace $g(x)$ by $\max\big(g(y), g(x)\big)$ and regularize this to

$$\widetilde{g}(x) \;=\; \int ds\, \delta(s)\big[s\theta\big(s - g(x)\big) + g(x)\theta\big(g(x) - s\big)\big]\,,$$

where $0 \le \delta \in C_0^\infty(R)$ is a regularized δ-distribution supported near $g(y)$. By construction $\widetilde{g}$ is a Yafaev function with Hessian

$$\widetilde{g}''(x) \;=\; \sigma^2\big(1_a - \pi_a(x)\big)\delta\big(g(x)\big) + \frac{\sigma}{|x_a|}\,\pi_a \int_{-\infty}^{g(x)} ds\, \delta(s)\ , \qquad (A.11)$$

which is strictly positive near y. Multiplying $\widetilde{g}$ with a suitable constant we thus have $\pm f''(x) \le \widetilde{g}''(x)$ in some neighbourhood of y. Since the Yafaev functions form a positive cone this estimate extends to all x in the compact shell $R_1 \le |x| \le R_2$ by summing over finitely many local bounds. The resulting estimate then extends to $|x| > R_2$ by scaling $x \to \lambda x$ $(\lambda > 0)$. In fact (A.11) implies

$$g''(\lambda x) \ge \text{const.}\, \frac{\pi_a(x)}{\lambda |x_a|}\ , \quad \text{while} \quad \pm f''(\lambda x) \le \text{const.}\, \frac{\pi_a(x)}{\lambda |x_a|}$$

by homogeneity. For $|x| < R_1$ $f''(x) = 0$ so that (A.10) is trivial. □

B. COMMUTATOR EXPANSIONS

Functions of selfadjoint operators. A convenient operator calculus for functions $f(A)$ of selfadjoint operators A can be based on a formula given by Helffer–Sjöstrand [HelSjo] :

$$f(A) = -\frac{1}{2\pi} \int_{R^2} (z - A)^{-1}\ \partial_{\bar z} \widetilde{f}(z)\ dx\, dy, \qquad (B.1)$$

where $z = x + iy$; $\partial_{\bar z} = \partial_x + i\partial_y$. Here f is some given complex function on R, and $\widetilde{f}$ a largely arbitrary extension of f to the complex plane, which must be *almost analytic* in the sense that it satisfies the Cauchy–Riemann equations on the real axis:

$$\partial_{\bar z} \widetilde{f}(z) = 0 \ \mathit{for}\ z \in R. \qquad (B.2)$$

We abbreviate (B.1) by writing:

$$f(A) = \int d\widetilde{f}(z)\,(z-A)^{-1}; \quad d\widetilde{f}(z) \equiv -\frac{1}{2\pi}\,\partial_{\bar z}\widetilde{f}(z)\;dx\,dy. \tag{B.3}$$

For example, if $f \in C_0^2(R)$, we can construct the almost analytic extension

$$\widetilde{f}(z) = \big(f(x) + iyf'(x)\big)\;\chi(z) \tag{B.4}$$

in $C_0^1(C)$ by taking $\chi \in C_0^\infty(C)$ with $\chi = 1$ on some complex neighbourhood of supp(f).

Lemma B.1. *(B.3) holds for $f \in C_0^2(R)$ if $\widetilde{f} \in C_0^1(C)$ is an almost analytic extension of f, the integral being absolutely convergent in norm sense.*

Proof. $\partial_{\bar z}\widetilde{f}$ has compact support and vanishes on the real axis, so that $|\partial_{\bar z}\widetilde{f}(z)| \le$ const. $|y|$. On the other hand, $\|(z-A)^{-1}\| \le |y|^{-1}$. Therefore the integral (B.3) converges absolutely in norm sense, and it suffices to prove that

$$f_\epsilon(t) \equiv \int_{|y|>\epsilon} d\widetilde{f}(z)\,(z-t)^{-1}$$

converges pointwise to $f(t)$ for $t \in R$ as $\epsilon \searrow 0$. Since $(z-t)^{-1}$ is analytic for $z \notin R$ we have $\partial_{\bar z}\,(z-t)^{-1} = 0$. Therefore we obtain after partial integrations in x and y:

$$f_\epsilon(t) = \int dx\, g_\epsilon(t,x); \quad g_\epsilon(t,x) = \frac{1}{2\pi i}\widetilde{f}(x+iy)(x+iy-t)^{-1}\Big|_{y=\epsilon}^{y=-\epsilon}.$$

Expanding $\widetilde{f}(x \pm i\epsilon) = f(x) \pm i\epsilon f'(x) + O(\epsilon^2)$ we find:

$$g_\epsilon(t,x) = \frac{1}{\pi}f(x)\frac{\epsilon}{(x-t)^2+\epsilon^2} - \frac{1}{2\pi}f'(x)\frac{2\epsilon(x-t)}{(x-t)^2+\epsilon^2} + O(\epsilon).$$

The second term is bounded by $(1/2\pi)|f'(x)|$ and vanishes pointwise for $x \neq t$ as $\epsilon \to 0$. Therefore

$$\lim_{\epsilon\searrow 0} f_\epsilon(t) = \lim_{\epsilon\searrow 0}\frac{1}{\pi}\int dx\, f(x)\,\frac{\epsilon}{(x-t)^2+\epsilon^2} = f(t). \qquad \square$$

Now let $f \in C^{n+2}(R)$ for some $n \geq 0$. Following [IvrSig] (see also [Dav]) we generalize (B.4) by constructing the almost analytic extension

$$\widetilde{f}(z) = \chi\left(\frac{y}{\langle x\rangle}\right)\sum_{k=0}^{n+1} f^{(k)}(x)\frac{(iy)^k}{k!}, \tag{B.5}$$

where $\langle x\rangle = (1+x^2)^{1/2}$; $\chi \in C_0^\infty(R)$ and $\chi = 1$ on some open interval $\ni 0$. ¿From

$$\partial_{\bar z}\sum_{k=0}^{n+1} f^{(k)}(x)\frac{(iy)^k}{k!} = f^{(n+2)}(x)\frac{(iy)^{n+1}}{(n+1)!};$$

$$\partial_{\bar z}\,\chi\left(\frac{y}{\langle x\rangle}\right) = \frac{1}{\langle x\rangle}\chi'\left(\frac{y}{\langle x\rangle}\right)\left(i - \frac{xy}{\langle x\rangle^2}\right)$$

we obtain the estimate:

$$|\partial_{\bar z}\widetilde{f}(z)| \leq \left|\chi\left(\frac{y}{\langle x\rangle}\right)\frac{(iy)^{n+1}}{(n+1)!}\right|\,\left|f^{(n+2)}(x)\right| + \sum_{k=0}^{n+1}\left|\rho\left(\frac{y}{\langle x\rangle}\right)\frac{y^k}{k!}\right|\,\left|\frac{1}{\langle x\rangle}f^{(k)}(x)\right|, \tag{B.6}$$

where $\rho(t) = |\chi'(t)|\,\langle t\rangle$ has compact support $\not\ni 0$. Therefore:

$$\int dy\,|\partial_{\bar z}\widetilde{f}(z)|\,|y|^{-p-1} \leq \text{const.}\sum_{k=0}^{n+2}\langle x\rangle^{k-p-1}\left|f^{(k)}(x)\right|,$$

since the integrability of the first term in (B.6) against $|y|^{-p-1}$ requires $p \leq n$. Defining the norms

$$\|f\|_m = \int dx\,\langle x\rangle^m\,|f(x)| \tag{B.7}$$

we obtain

$$\int |d\widetilde{f}(z)|\,|Im(z)|^{-p-1} \leq \text{const.}\sum_{k=0}^{n+2}\|f^{(k)}\|_{k-p-1} \tag{B.8}$$

for $p = 0\ldots n$, provided that

$$\|f^{(k)}\|_{k-p-1} < \infty \textit{ for } k = 0\ldots n+2. \tag{B.9}$$

Lemma B.2. *Let $f \in C^{n+2}(R)$, $n \geq 0$, and suppose that (B.9) holds for $p = 0\ldots n$. Let $\widetilde{f}(z)$ be given by (B.5). Then*

$$\frac{1}{p!}f^{(p)}(A) = \int d\widetilde{f}(z)\,(z-A)^{-p-1} \tag{B.10}$$

for $p = 0 \dots n$ and for all selfadjoint operators A, where by (B.8) the integral converges absolutely in norm sense and is bounded uniformly in A.

Proof. To prove (B.10) we first assume $f \in C_0^{n+2}(R)$. Then $\partial_x^p \widetilde{f}(z)$ is an almost analytic extension of $f^{(p)}(x)$ in the sense of Lemma B.1, so that

$$f^{(p)}(A) = \int d\widetilde{f}(z)\ (z-A)^{-1} = p! \int d\widetilde{f}(z)\ (z-A)^{-p-1}$$

by partial integration in x. Now let $f \in C^{n+2}(R)$ obey (B.9). Then (B.10) holds for f replaced by $f_m(x) = f(x)\chi(x/m)$, $\chi \in C_0^\infty(R)$ with $\chi(x) = 1$ near $x = 0$. It is easy to see that

$$\lim_{m\to\infty} \|f^{(k)} - f_m^{(k)}\|_{k-p-1} = 0; \quad k = 0 \dots n+2.$$

Moreover, $f_m^{(p)}(x)$ is uniformly bounded in terms of $\|f_m^{(p+1)}\|_0$ and converges pointwise to $f^{(p)}(x)$ as $m \to \infty$. Therefore (B.10) is preserved in this limit. $\square$

Commutator Expansions. Now we derive expansion formula for commutators with remainder whose prototype was introduced in [SigSof2] (see also [AmBoGe] for a different version). We consider two bounded operators H and $A = A^*$. Multiple commutators are defined recursively by

$$ad_A^{(k)}(H) = \left[ad_A^{(k-1)}(H), A\right]; \quad ad_A^{(0)}(H) = H.$$

Then

$$[H, (z-A)^{-1}] = (z-A)^{-1}[H, A](z-A)^{-1}, \tag{B.11}$$

and more generally:

$$\left[ad_A^{(k-1)}(H), (z-A)^{-1}\right] = (z-A)^{-1} ad_A^{(k)}(H)(z-A)^{-1}. \tag{B.12}$$

Starting from (B.11) we use (B.12) to commute the rightmost resolvent $(z-A)^{-1}$ systematically to the left, obtaining:

$$[H, (z-A)^{-1}] = \sum_{k=1}^{n-1} (z-A)^{-k-1} ad_A^{(k)}(H) + (z-A)^{-n} ad_A^{(n)}(H)(z-A)^{-1}. \tag{B.13}$$

Let $f \in C_0^\infty(R)$, and let $\widetilde{f}$ be the almost analytic extension (B.5). From (B.13) and Lemma B.2 we find the commutator expansion:

$$\begin{aligned} [H, f(A)] &= \sum_{k=1}^{n-1} \frac{1}{k!} f^{(k)}(A)\, ad_A^{(k)}(H) + R_n; \\ R_n &= \int d\widetilde{f}(z)(z-A)^{-n} ad_A^{(n)}(H)(z-A)^{-1} \end{aligned} \tag{B.14}$$

with the estimate

$$\|R_n\| \leq \text{const.}\, \|ad_A^{(n)}(H)\| \sum_{k=0}^{n+2} \|f^{(k)}\|_{k-n}\,. \tag{B.15}$$

Similarly, we could have commuted the resolvents $(z-A)^{-1}$ systematically to the right, arriving at

$$\begin{aligned} [H, f(A)] &= \sum_{k=1}^{n-1} \frac{1}{k!} (-1)^{k-1} ad_A^{(k)}(H)\, f^{(k)}(A) + R_n; \\ R_n &= (-1)^{n-1} \int d\widetilde{f}(z)(z-A)^{-1} ad_A^{(n)}(H)(z-A)^{-n} \end{aligned} \tag{B.16}$$

and with the same estimate (B.15). Combining the two expansions we also find a useful symmetric form for $n = 2$:

$$[H, f(A)] = \frac{1}{2}\left[f'(A)\, ad_A^{(1)}(H) + ad_A^{(1)}(H)\, f'(A)\right] + R_2; \tag{B.17}$$

$$\begin{aligned} R_2 &= \frac{1}{2}\int d\widetilde{f}(z)(z-A)^{-1}\left[(z-A)^{-1}, ad_A^{(2)}(H)\right](z-A)^{-1} \\ &= -\frac{1}{2}\int d\widetilde{f}(z)(z-A)^{-2}\, ad_A^{(3)}(H)\,(z-A)^{-2}. \end{aligned} \tag{B.18}$$

As in the proof of Lemma 1, these expansions extend to all bounded C^∞–functions f with bounded derivatives, as long as the norms arising in (B.15) remain finite.

Commutator Estimates. We will often deal with commutators of the form $[g(H), f(A)]$ for unbounded selfadjoint operators H, A. We assume that $g \in C_0^\infty(R)$. Then the representation

$$[g(H), A] = \int d\widetilde{g}(z)(z-H)^{-1}[H, A](z-H)^{-1} \tag{B.19}$$

requires an almost analytic extension $\widetilde{g}(z)$ of the form (B.5) with $n \geq 1$. The integral is well defined if $[H, A]$ is H–bounded, since then

$$\|[H, A](z-H)^{-1}\| \leq \text{const.}\,(1+|z|)|Im(z)|^{-1},$$

where the factor $|z|$ is harmless since $\widetilde{g}$ has compact support. Similarly, we can deal with

$$ad_A^{(k)}(g(H)) = \int d\widetilde{g}(z)\, ad_A^{(k)}((z-H)^{-1}), \tag{B.20}$$

writing out

$$\begin{aligned} ad_A^{(1)}((z-H)^{-1}) =& (z-H)^{-1} ad_A^{(1)}(H)(z-H)^{-1}; \\ ad_A^{(2)}((z-H)^{-1}) =& 2(z-H)^{-1} ad_A^{(1)}(H)(z-H)^{-1} ad_A^{(1)}(H)(z-H)^{-1} \\ &+ (z-H)^{-1} ad_A^{(2)}(H)(z-H)^{-1}; \end{aligned}$$

and so forth. Therefore, if $ad_A^{(k)}(H)$ is H–bounded for $1 \leq k \leq n$, we have

$$\|ad_A^{(n)}((z-H)^{-1})\| \leq \text{const.} \sum_{p=1}^{n} |Im(z)|^{-p-1}$$

on $\text{supp}(\widetilde{g})$. To use (B.20) we take an almost analytic extension $\widetilde{g}(z)$ of the form (B.5) for the given n, which leads to a bound:

$$\|ad_A^{(n)}(g(H))\| \leq \text{const.} \sum_{p=1}^{n} \sum_{k=0}^{n+2} \|g^{(k)}\|_{k-p-1}. \tag{B.21}$$

Now we can discuss

$$[g(H), f(A)] = \int d\widetilde{f}(z)(z-A)^{-1}[g(H), A](z-A)^{-1}. \tag{B.22}$$

If $[H, A]$ is H–bounded, then $[g(H), A]$ is bounded. $\widetilde{f}(z)$ can be taken of the form (B.5) with $n = 1$, and the convergence of the integral (B.22) requires that

$$\|f^{(k)}\|_{k-2} < \infty \;\; for \;\; k = 0 \ldots 3. \tag{B.23}$$

This already allows $f(x)$ to grow like $|x|^p$ with $p < 1$, if also $f^{(k)}(x) = O(|x|^{p-k})$ for $k \leq 3$. Suppose now that $ad_A^{(k)}(H)$ is H–bounded for $k \leq n$. Then $ad_A^{(k)}(g(H))$ is bounded for $k \leq n$ and we can represent the commutator $[g(H), f(A)]$ by an expansion, like

$$\begin{aligned} [g(H), f(A)] &= \sum_{k=1}^{n-1} \frac{1}{k!} f^{(k)}(A) ad_A^{(k)}(g(H)) + R_n; \\ R_n &= \int d\widetilde{f}(z)(z-A)^{-n} ad_A^{(n)}(g(H))(z-A)^{-1}. \end{aligned} \qquad (B.24)$$

Here $\widetilde{f}(z)$ must be of the form (B.5) for the given n, but the convergence of the integral only requires that

$$\|f^{(k)}\|_{k-n-1} < \infty \ for \ k = 0 \ldots n+1. \qquad (B.25)$$

This allows $f(x)$ to grow like $|x|^p$, $p < n$, with corresponding slower growth of the derivatives.

C. ESTIMATES FOR THE LONG RANGE CASE

Here we derive additional propagation estimates for the dynamics $U_t: \quad \psi \to \psi_t$ generated by $H_t = H + W_t(x)$. These estimates are used in section 8 and (indirectly) in section 9. They are based on the hypothesis

$$\begin{aligned} &\nabla I_a(x) = O(|x|_a^{-\mu-1}); \\ &\nabla W_t(x) =\leq \text{const.}(1+|x|)^{-\mu-1} \quad \forall t. \end{aligned} \qquad (\mu > 0) \qquad (C.1))$$

Roughly speaking we show that the region of ballistic motion can be decoupled from that of a subballistic one (Theorem C.2 and its consequence). This is used in section 8 in order to conclude that the subballistic part of any orbit is a bound state of H.

We pick the scaling parameters δ and δ' in the ranges

$$\frac{2}{3} < \delta < 1; \quad \delta(\mu+2) > 2, \qquad \delta < \delta' < 1. \qquad (C.2)$$

We also define

$$\begin{aligned} \Gamma_t &:= \gamma_t - \partial_t g_t = \frac{1}{2}(\nabla g_t \cdot p + p \cdot \nabla g_t); \\ K &:= \frac{1}{2}p^2 + 1; \quad \|\psi\|_H := \|\psi\| + \|H\psi\|, \end{aligned} \qquad (C.3)$$

and we will use (1.16) to estimate $\|K\psi_t\| \le \text{const.}\|\psi\|_H$. With $\chi(x \le \theta)$ we denote any smoothed characteristic function of the type shown in Fig. 6; in particular $\text{supp}(\chi) \subset (-\infty, \theta]$ and $0 \ge \chi' \in C_0^\infty(R)$.

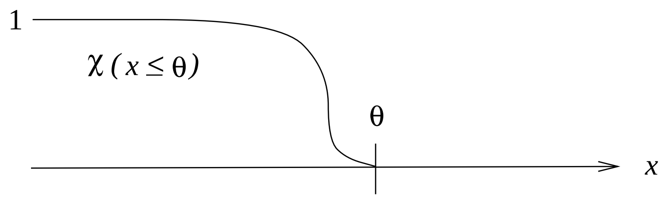

Fig. 6

If A is a selfadjoint operator then $\chi(A \le \theta)$ is the corresponding "function" of A, and $\chi(A \ge \theta)$ is defined analogously. To estimate commutators involving such operators we will use the methods of Appendix B. The results of this appendix are:

Theorem C.1. *Let $0 < \theta_1 \le \theta$. Then, for large t and all $\psi \in D(H)$*

$$\begin{aligned} &\|\chi(t^{1-\delta'}\Gamma_t \le \theta_1)\,\chi(t^{-\delta'}g_t \ge \theta)\,\psi_t\|^2 \\ &\quad \le \|\chi(t^{-\delta'}g_t \ge \theta)\,\psi\|^2 + \text{const.}t^{-\rho}\|\psi\|_H^2 \quad (\rho > 0). \end{aligned} \tag{C.4}$$

Remark: $\delta' > \delta$ implies that $\chi(t^{-\delta'}g_t \ge \theta) \to 0$ strongly as $t \to \infty$. Therefore it follows from (C.4) that

$$\lim_{t\to\infty} \chi(t^{1-\delta'}\Gamma_t \le \theta_1)\,\chi(t^{-\delta'}g_t \ge \theta)\,\psi_t = 0.$$

This is equivalent to

$$\lim_{t\to\infty} \chi(t^{-\delta'}g_t \ge \theta)\,\chi(t^{1-\delta'}\Gamma_t \le \theta_1)\,\psi_t = 0 \tag{C.5}$$

$$\text{since} \qquad \|\,[t^{1-\delta'}\Gamma_t, t^{-\delta'}g_t]\,\| \le \text{const.}\, t^{1-2\delta'} \to 0. \tag{C.6}$$

Theorem C.2. *Let $\theta > 0$. Then for large t*

$$D_t\,\chi(t^{-\delta'}g_t \ge \theta) = \sum_{k=1}^{6} \pm B_k(t) + O(t^{-\rho}) \tag{C.7}$$

in form sense on $D(H)$, with an appropriate sign $\pm$ for each k. The quadratic forms $B_k(t)$ are positive and satisfy

$$\int_1^\infty dt\,\langle B_k(t)\rangle_t \le \text{ const. } \|\psi\|_H^2 \quad \forall\psi \in D(H). \tag{C.8}$$

The symbol $O(t^{-\rho})$ denotes a form on $D(H)$ with

$$|\langle O(t^{-\rho})\rangle_\psi| \le \text{ const. } t^{-\rho}\,\|\psi\|_H^2 \quad (\rho > 1) \tag{C.9}$$

for large t and all $\psi \in D(H)$.

Proofs. To prepare the proof of Theorem C.1 we introduce a variable $s \in R^+$ and we consider the form

$$\Phi_t(s) = f\chi f; \quad f = f\big(s^{-\delta'}(g_s - ct)\big); \quad \chi = \chi(b\Gamma_s), \tag{C.10}$$

on $D(H)$, with real parameters $b > 0$ and c to be adjusted later as functions of s. f and χ are smooth characteristic functions depicted in Fig. 7:

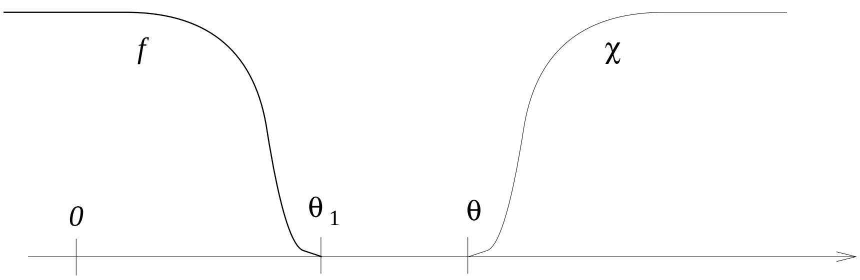

Fig. 7

Our strategy is to estimate the form

$$D_t\,\Phi_t(s) = f(D_t\chi)f + \big((D_tf)\chi f + \text{adjoint}\big). \tag{C.11}$$

for $0 \le t \le s$ (s large), and then to use this estimate to derive the desired bound for

$$\langle\Phi_s(s)\rangle_s = \langle\Phi_0(s)\rangle_0 + \int_0^s dt\,\langle D_t\Phi_t(s)\rangle_t. \tag{C.12}$$

Lemma C.3. *For s sufficiently large and for all $\psi \in D(H)$*

$$\langle D_t \chi \rangle_\psi \leq \text{ const. } (b^3 s^{-3\delta} + b s^{-\delta(\mu+1)}) \, \|\psi\|_H^2 \tag{C.13}$$

uniformly in t.

Proof. We write

$$D_t \chi = i[H_t, \chi] = A + B; \qquad A = i[K, \chi]; \qquad B = i[V + W_t, \chi]. \tag{C.14}$$

Estimate of A: the symmetric expansion (B.18) for $K^{-1} A K^{-1} = -i[K^{-1}, \chi]$ reads

$$\begin{aligned} K^{-1} A K^{-1} =& -\frac{b}{2}(\chi' i[K^{-1}, \Gamma_s] + \text{ adjoint}) \\ &+ \frac{ib^3}{2} \int d\widetilde{\chi}(z) \, (z - b\Gamma_s)^{-2} \, ad^{(3)}_{\Gamma_s}(K^{-1}) \, (z - b\Gamma_s)^{-2}. \end{aligned} \tag{C.15}$$

To estimate these terms we note that

$$ad^{(k)}_{\Gamma_s}(K) = p_m \, G^{(k)}_{mn}(x) \, p_n + G^{(k)}(x),$$

where $G^{(k)}_{mn}(x)$ and $G^{(k)}(x)$ are polynomials of derivatives of $g_s(x)$, supported in $\{|x| \geq s^\delta\}$ and homogeneous in x of degree $-k$ and $-(k+2)$, respectively, for large $|x|$. This leads to

$$\begin{aligned} \|K^{-1} \, ad^{(k)}_{\Gamma_s}(K) \, K^{-1}\| &\leq \text{ const. } s^{-k\delta} \quad \text{and} \\ \|ad^{(k)}_{\Gamma_s}(K^{-1})\| &\leq \text{ const. } s^{-k\delta}. \end{aligned} \tag{C.16}$$

Therefore the second term in (C.15) is of order $b^3 s^{-3\delta}$ in norm as $s \to \infty$. The first term is symmetrized using $\chi' \leq 0$ and

$$\begin{aligned} -\frac{1}{2}\chi' \, i[K^{-1}, b\Gamma_s] + \text{ adjoint} =& |\chi'|^{1/2} \, i[K^{-1}, b\Gamma_s] \, |\chi'|^{1/2} \\ &+ \frac{1}{2}[\,|\chi'|^{1/2}, [\,|\chi'|^{1/2}, [i[K^{-1}, b\Gamma_s]\,]\,]. \end{aligned}$$

By (C.16)) the multiple commutator is of order $b^3 s^{-3\delta}$ in norm. Finally, using

$$i[K^{-1}, \Gamma_s] = -K^{-1} i[K, \Gamma_s] K^{-1} = -K^{-1} \, (p g_s'' p - \frac{1}{4}\Delta^2 g_s) \, K^{-1}$$

and $\Delta^2 g_s = O(s^{-3\delta})$ we arrive at

$$K^{-1}AK^{-1} = -Q + O(bs^{-3\delta} + b^3 s^{-3\delta})$$

in norm as $s \to \infty$, where

$$Q = b|\chi'|^{1/2} K^{-1}(pg''p)K^{-1}|\chi'|^{1/2} \geq 0.$$

Therefore

$$\langle A \rangle_\psi = -\langle P \rangle_\psi + O(bs^{-3\delta} + b^3 s^{-3\delta}) \|\psi\|_H^2 \tag{C.17}$$

on $D(H)$, where $P = KQK$ is a positive quadratic form.

Estimate of B: By (C.1) the commutator in the representation

$$B = ib \int d\tilde{\chi}(z)(z - b\Gamma_s)^{-1} \left[V + W_t, \Gamma_s\right] (z - b\Gamma_s)^{-1}$$

is of order $s^{-\delta(\mu+1)}$ in norm. Therefore

$$\|B\| \leq \text{ const. } b\, s^{-\delta(\mu+1)} \tag{C.18}$$

uniformly in t if s is sufficiently large. (C.13) now follows from (C.17) and (C.18). □

Lemma C.4. *If $bc \geq \theta_1$ then*

$$\langle (D_t f)\chi f + \text{ adjoint} \rangle_\psi \leq \text{ const. } bs^{-2\delta'} \|\psi\|^2 \tag{C.19}$$

for all $\psi \in D(H)$, uniformly in t.

Proof. Since $f(s^{-\delta'}(g_s - ct))$ is a function of x we can easily compute $D_t(f)$ with the result

$$D_t f = s^{-\delta'} (f')^{1/2} \cdot (\Gamma_s - c) \cdot (f')^{1/2}, \tag{C.20}$$

where we have used that $f' \geq 0$ and that the commutator of Γ_s with a function of x is again a function of x. In particular, $i[\Gamma_s, g_s] = (\nabla g_s)^2$ is bounded uniformly in s so that

$$\| \left[(f')^{1/2}, \chi(b\Gamma_s)\right] \| \leq \text{ const. } bs^{-\delta'}.$$

Using this we arrive at

$$(D_t f)\chi = s^{-\delta'}\,(f')^{1/2}\,\chi(b\Gamma_s)\cdot(\Gamma_s - c)\cdot(f')^{1/2} + O(bs^{-2\delta'});$$

$$(D_t f)\chi f + \text{ adjoint} = s^{-\delta'}\,f_1\,\chi(b\Gamma_s)\cdot(\Gamma_s - c)\cdot f_1 + O(bs^{-2\delta'}), \qquad (C.21)$$

where $f_1^2 := (f^2)'$. (C.19) now follows by observing that $\chi(b\Gamma_s)\cdot(\Gamma_s - c) \le 0$ if $bc \ge \theta_1$. □

Proof of Theorem C.1. By (C.13) and (C.19)

$$\langle D_t \Phi_t(s)\rangle_t \le \text{ const. } (b^3 s^{-3\delta} + bs^{-\delta(\mu+1)})\|\psi\|_H^2$$

uniformly in t. From (C.12) we thus obtain

$$\langle \Phi_s(s)\rangle_s \le \langle \Phi_0(s)\rangle_0 + \text{ const. } (b^3 s^{1-3\delta} + bs^{1-\delta(\mu+1)})\|\psi\|_H^2. \qquad (C.22)$$

Now we fix $b = s^{1-\delta'}$; $\quad c = \theta_1\, s^{\delta'-1}$. Then (C.22) reads

$$\langle \Phi_s(s)\rangle_s \le \langle \Phi_0(s)\rangle_0 + \text{ const. } s^{-\rho}\,\|\psi\|_H^2,$$

where $\rho = \min(6\delta - 4, \delta(\mu+2) - 2) > 0$. Replacing s by t and χ by χ^2 we arrive at (C.6).

□

For the proof of Theorem C.2 we consider $f = f(t^{-\delta'} g_t)$ with the function f shown in Fig. 8.

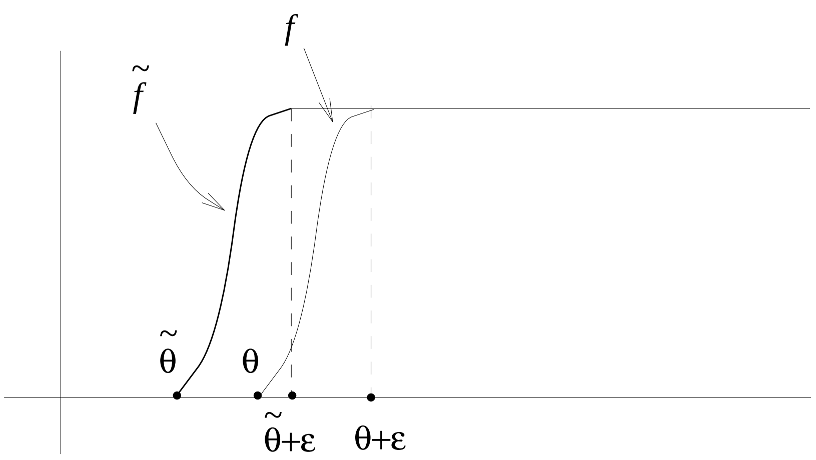

Fig. 8

Our task is to decompose $D_t(f^2)$ into a sum of positive and negative quadratic forms in the sense of (C.8). Like (C.20) we find

$$D_t(f^2) = t^{-1} f_1 \cdot (t^{1-\delta'}\Gamma_t - \delta' t^{-\delta'} g_t) \cdot f_1, \tag{C.23}$$

with $f_1^2 = (f^2)'$. The first step of the decomposition is achieved by inserting a partition of unity

$$1 = \sum_{k=1}^{3} \chi_k(t^{1-\delta'}\Gamma_t),$$

with functions χ_k as shown in Fig. 9.

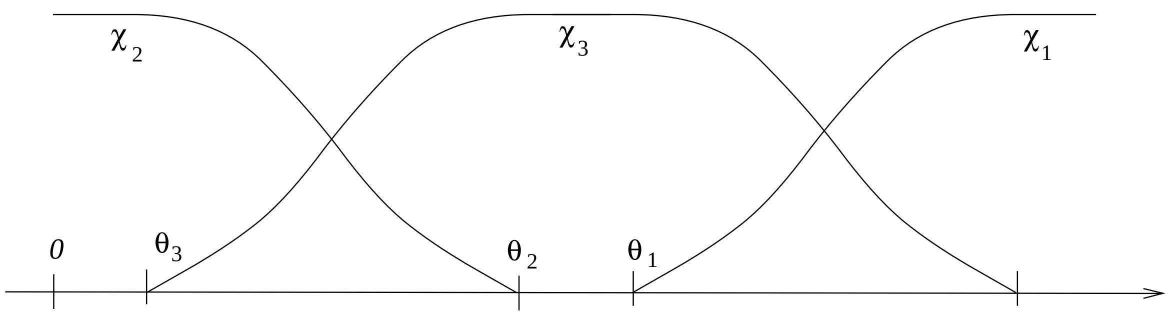

Fig. 9

The parameters $\theta_1\ \ldots\ \theta_3$ will be selected in the course of the proof. (C.6) allows us to write

$$D_t(f^2) = \sum_{k=1}^{3} t^{-1} f_1\, \chi_k^{1/2} \cdot (t^{1-\delta'}\Gamma_t - \delta' t^{-\delta'} g_t) \cdot \chi_k^{1/2}\, f_1 + O(t^{-\rho}), \tag{C.24}$$

with $O(t^{-\rho})$ defined in (C.9). For the same reason the factors $\chi_k^{1/2}$ and f_1 can be freely commuted modulo contributions to $O(t^{-\rho})$. The task is now reduced to prove (C.7) separately for each term in the sum (C.24). As a preparation we estimate the form

$$D_t(f\chi f) = f(D_t\chi)f + \big((D_t f)\chi f + \text{ adjoint}\big),$$

$\chi = \chi(t^{1-\delta'}\Gamma_t)$, where χ is one of the functions χ_1, χ_2. Since $\chi_1' \leq 0$ and $\chi_2' \geq 0$ we distinguish the two cases:

Lemma B.5. *Let $\pm\chi' \geq 0$. Then, correspondingly,*

$$f(D_t\chi)f = \pm P \pm (1-\delta')\, t^{-1}\, f\,|\chi'|\, t^{1-\delta'}\Gamma_t\, f + O(t^{-\rho}), \tag{C.25}$$

where P is a positive quadratic form on $D(H)$ and $O(t^{-\rho})$ is defined by (C.9).

Proof. The proof is essentially the same as the proof of Lemma C.3. Compared with (C.14) we now have

$$D_t\chi = A + B + C$$

with the additional term

$$C = \chi'\partial_t(t^{1-\delta'}\Gamma_t) = (1-\delta')\, t^{-\delta'}\, \chi'\Gamma_t + t^{1-\delta'}\, \chi'\partial_t\Gamma_t.$$

We note that

$$f\chi'\,(\partial_t\Gamma_t)\, f = 0$$

for large t since then $\partial_t g_t = 0$ on the support of f. The contributions of A and B are estimated as in the proof of Lemma C.3, replacing s by t, b by $t^{1-\delta'}$, and taking the sign of χ' into account. Corresponding to (C.13) the resulting error term is of order $t^{-\rho}$ with $\rho = \min(6\delta - 3, \delta(\mu+2) - 1) > 1$. □

Lemma C.6. *let $f_1^2 = (f^2)'$. Then*

$$(D_t f)\chi f + \text{ adjoint} = t^{-1}\, f_1\, \chi^{1/2} \cdot (t^{1-\delta'}\Gamma_t - \delta' t^{-\delta'} g_t) \cdot \chi^{1/2}\, f_1 + O(t^{-\rho}). \tag{C.26}$$

Proof. This estimate corresponds to (C.21). The only difference in the proof is that now

$$\partial_t f = -\delta' t^{-1-\delta'}\, f' g_t + t^{-\delta'}\, f'\partial_t g_t,$$

where the last term vanishes exactly for large t. □

Proof of Theorem C.2. By the results so far we have for $\pm\chi' \geq 0$:

$$
\begin{aligned}
D_t(f\chi f) = &\pm P && (P \geq 0)\\
&\pm (1-\delta')\, t^{-1}\, f\, |\chi'| \cdot (t^{1-\delta'}\Gamma_t) \cdot f\\
&+ t^{-1}\, f_1\, \chi^{1/2} \cdot (t^{1-\delta'}\Gamma_t - \delta' t^{-\delta'} g_t) \cdot \chi^{1/2}\, f_1\\
&+ O(t^{-\rho}) && (\rho > 1).
\end{aligned}
\tag{C.27}
$$

Now we can decompose each term of the sum (C.24) in the sense of (C.7):

Term (k=1): Since $\chi_1' \leq 0$ and $|\chi_1'| t^{1-\delta'}\Gamma_t \geq 0$ we obtain from (C.27)

$$
\begin{aligned}
D_t(f\chi_1 f) &\leq t^{-1}\, f_1\, \chi_1^{1/2} \cdot (t^{1-\delta'}\Gamma_t - \delta' t^{-\delta'} g_t) \cdot \chi_1^{1/2}\, f_1 + O(t^{-\rho})\\
&= -t^{-1}\, f_1\, \chi_1 \cdot (\theta_1 - t^{1-\delta'}\Gamma_t) \cdot f_1\\
&\quad - t^{-1}\, \chi_1^{1/2}\, f_1 \cdot (\delta' t^{-\delta'} g_t - \theta_1) \cdot f_1\, \chi_1^{1/2} + O(t^{-\rho}).
\end{aligned}
\tag{C.28}
$$

We observe that $\chi_1 \cdot (\theta_1 - t^{1-\delta'}\Gamma_t) \geq 0$ due to the support of χ_1. Since

$$\theta \leq t^{-\delta'} g_t \leq \theta + \epsilon$$

on $\mathrm{supp}(f_1)$, we also have $f_1 \cdot (\delta' t^{-\delta'} g_t - \theta_1) \cdot f_1 \geq 0$ by choosing $0 < \theta_1 < \delta'\theta$. Now (C.28) shows that the two positive quadratic forms

$$
\begin{aligned}
B_1 &:= t^{-1} f_1 \chi_1 \cdot (\theta_1 - t^{1-\delta'}\Gamma_t) \cdot f_1;\\
B_2 &:= t^{-1} \chi_1^{1/2} f_1 \cdot (\delta' t^{-\delta'} g_t - \theta_1) \cdot f_1 \chi_1^{1/2}
\end{aligned}
\tag{C.29}
$$

are integrable in the sense of (C.8), and that

$$\textit{Term}\ (k=1) = -B_1 - B_2 + O(t^{-\rho}).$$

Term (k=2): Choosing $\theta_2 > \delta'(\theta + \epsilon)$ we find in the same way

$$
\begin{aligned}
&\textit{Term}\ (k=2) = B_3 + B_4 + O(t^{-\rho}),\\
&\qquad B_3 := t^{-1} f_1 \chi_2^{1/2} \cdot \left(t^{1-\delta'}\Gamma_t - \theta_2\right) \cdot \chi_2^{1/2}\ f_1;\\
&\qquad B_4 := t^{-1} \chi_2^{1/2} \cdot \left(\theta_2 - \delta' t^{-\delta'} g_t\right) \cdot\ f_1\, \chi_2^{1/2}.
\end{aligned}
\tag{C.30}
$$

In addition we also conclude from (C.27) that

$$D_t(f\chi_2 f) \geq (1-\delta')\,t^{-1}\,f\,\chi_2'\cdot(t^{1-\delta'}\Gamma_t)\cdot f + O(t^{-\rho}),$$

which gives

$$\int_1^\infty dt\; t^{-1}\,\langle f\,\chi_2'\,t^{1-\delta'}\Gamma_t\,f\rangle_t \leq \text{ const.}\,\|\psi\|_H^2. \tag{C.31}$$

Term (k=3): Here we exploit (C.31) and the fact that

$$\widetilde{\chi}_2(x) := \int_{-\infty}^x ds\,\chi_3(s)$$

has the same general form as χ_2, but with support $[\theta_3, +\infty)$. Hence, replacing f by a function $\widetilde{f}$ shown in Fig. 8 such that $\theta_3 > \delta'(\widetilde{\theta}+\epsilon)$, (C.31) takes the form:

$$\int_1^\infty dt\; t^{-1}\,\langle \widetilde{f}\,\chi_3\,t^{1-\delta'}\Gamma_t\,\widetilde{f}\rangle_t \leq \text{ const.}\,\|\psi\|_H^2. \tag{C.32}$$

Since $\widetilde{\theta} < \theta$ we also have $f_1 \leq$ const. $\widetilde{f}$, so that

$$f_1\,\chi_3\cdot\left(t^{1-\delta'}\Gamma_t\right)\cdot f_1 \leq \text{ const. } \widetilde{f}\chi_3\cdot\left(t^{1-\delta'}\Gamma_t\right)\cdot\widetilde{f} + O(t^{-\rho}).$$

Therefore (C.32) implies

$$\int_1^\infty dt\; t^{-1}\,\langle f_1\,\chi_3\cdot(t^{1-\delta'}\Gamma_t)\cdot f_1\rangle_t \leq \text{ const.}\,\|\psi\|_H^2.$$

and since $\chi_3\cdot(t^{1-\delta'}\Gamma_t) \geq \theta_3\chi_3$:

$$\int_1^\infty dt\,t^{-1}\,\langle\, f_1\,\chi_3\,f_1\rangle_t \leq \text{ const.}\,\|\psi\|_H^2;$$

$$\int_1^\infty dt\,t^{-1}\langle\chi_3^{1/2}\,f_1\cdot(t^{-\delta'}g_t)\cdot f_1\,\chi_3^{1/2}\rangle_t \leq \text{ const.}\,\|\psi\|_H^2.$$

As a result:

$$\begin{aligned} \textit{Term }(k=3) &= B_5 - B_6 + O(t^{-\rho}); \\ B_5 &:= t^{-1}f_1\chi_3\cdot(t^{1-\delta'}\Gamma_t)\cdot\, f_1; \\ B_6 &:= t^{-1}\chi_3^{1/2}\,f_1\cdot(\delta' t^{-\delta'}g_t)\cdot f_1\,\chi_3^{1/2}. \end{aligned} \tag{C.33}$$

This concludes the proof of Theorem C.2. □

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