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ÉQUATIONS AUX DÉRIVÉES PARTIELLES

ASYMPTOTIC COMPLETENESS FOR N-BODY SHORT-RANGE QUANTUM SYSTEMS

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Asymptotic completeness for N -body short-range quantum systems

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Abstract. We give a sketch of a geometrical proof of asymptotic completeness for an arbitrary number of quantum particles interacting through short-range pair potentials. It relies on an estimate showing that the center of mass motion of clusters of particles concentrates asymptotically on classical trajectories. Full details can be found in [9].

1. Introduction

The first task of quantum scattering theory is to give a classification of the possible large time behaviours of Schrödinger orbits $e^{-itH}\psi$. In this contribution we study this problem for an arbitrary number of particles interacting via short range interactions. In the intuitive picture of the scattering process, this system is well described at large times by a number of bound clusters which do not feel each other, i.e. by free composite particles. This statement is called asymptotic completeness. For $N = 2, 3$ it was proved by several authors (see [1], Section 5.7 for a review), and in particular using geometric ideas by Enss [4], [5], [6]. For arbitrary N the proof is due to Sigal and Soffer [15].

The physical space is $\mathbb{R}^\nu$, $\nu \geq 1$. The configuration space of N mass points $m_i > 0$ in the center of mass (CM-) frame is the real vector space

$$X := \left\{ x = (x^1, \dots, x^N) \mid x^i \in \mathbb{R}^\nu, \sum_{i=1}^N m_i x^i = 0 \right\}$$

equipped with the metric

$$x \cdot y := 2 \sum_{i=1}^N m_i x^i \cdot y^i \quad ,$$

where $x^i \cdot y^i$ is the scalar product on $\mathbb{R}^\nu$. We will also use the notation $x^2 = x \cdot x$. The Hilbert space of the quantum mechanical N -body system is $\mathcal{H} = L^2(X)$, where the volume element of X is defined by the metric.

The Hamiltonian of the N -particle system is

$$H = p^2 + V := p^2 + \sum_{(ij)} V_{ij}(x^i - x^j) \tag{1.1}$$

on $L^2(X)$, where $p^2 = -\Delta$, and Δ is the Laplacian on X . We will come back to this and to other statements concerning the Hamiltonians at the end of this section. A cluster decomposition is a partition of $\{1, \dots, N\}$ into disjoint, nonempty subsets, called clusters.

The intercluster interactions for a cluster decomposition a is defined as the sum of all potentials linking different clusters in a , i.e. as

$$I_a := \sum_{(ij) \not\subset a} V_{ij}(x^{(ij)}) \quad ,$$

where $(ij) \not\subset a$ means that i, j belong to different cluster in a . Non-interacting clusters of a are the described by the Hamiltonian $H_a = H - I_a$. It decomposes naturally into a part describing the center of mass motion of the clusters in a , and an internal part H^a , whose bound state projection is denoted P^a . States in the range of P^a represent, physically speaking, a set of composite particles, each of them consisting of the ‘elementary’ particles of some cluster of a .

We say that the N -body short-range system above is *asymptotically complete*, if for any state $\psi \in L^2(X)$ and any $\varepsilon > 0$ there are states $\psi^a = P^a \psi^a \in L^2(X)$ such that

$$\left\| e^{-itH} \psi - \sum_a e^{-itH_a} \psi^a \right\| \leq \varepsilon$$

for $t > 0$ large enough. See [15] for a similar but equivalent definition.

We assume that the pair potentials are real and satisfy

Decay assumption:

$$\|F(|y| > R) V_{ij}(y) (p^2 + 1)^{-1}\| \leq \text{const } R^{-\mu_1} \quad , \quad (1.2)$$

$$\|F(|y| > R) \nabla V_{ij}(y) (p^2 + 1)^{-1}\| \leq \text{const } R^{-(1+\mu_2)} \quad (1.3)$$

for $R > R_0$ and some $R_0, \mu := \min(\mu_1, \mu_2) > 0$.

Short-range assumption:

$$\mu_1 > 1 \quad . \quad (1.4)$$

Compactness assumption:

$$V_{ij}(p^2 + 1)^{-1} \quad , \quad (p^2 + 1)^{-1} y \cdot \nabla V_{ij}(y) (p^2 + 1)^{-1} \quad \text{are compact.} \quad (1.5)$$

Here $p^2 = -\Delta$, and $F(|y| > R)$ is the characteristic function of the set $\{y \in \mathbb{R}^\nu \mid |y| > R\}$.

Theorem. *The quantum N -body system (1.1) satisfying (1.2)-(1.5) is asymptotically complete.*

Let us now introduce some further notion concerning N -body systems. For any cluster decomposition a we introduce the external configuration space

$$X_a := \left\{ x \in X \mid x^i = x^j \text{ if } i, j \in C \text{ for some } C \in a \right\} \quad ,$$

and its orthogonal complement, the internal configuration space

$$X^a := \left\{ x \in X \mid \sum_{i \in C} m_i x^i = 0 \text{ for } C \in a \right\} \quad .$$

The splitting $X = X_a \oplus X^a$ induces a decomposition $x =: x_a + x^a$, as well as the factorization

$$L^2(X) = L^2(X_a) \otimes L^2(X^a) \quad . \quad (1.6)$$

The dual of X is

$$X' = \left\{ k = (k_1, \dots, k_N) \mid k_i \in \mathbb{R}^\nu, \sum_{i=1}^N k_i = 0 \right\} \quad .$$

The particle momenta are the components of the operator p acting as $p\psi = (1/i)d\psi$, where d is the derivative. Hence its expectation values are in X' . Since the velocities are $v_i = p_i/m_i = 2p^i$, they are given by the contravariant components of the operator $2p$. The kinetic energy is then $\sum_i p_i^2/2m_i = \sum_i p_i p^i = p^2$.

With respect to the factorization (1.6) we have

$$H_a = (p_a)^2 \otimes \mathbf{1} + \mathbf{1} \otimes H^a \quad ,$$

with

$$H^a = (p^a)^2 + \sum_{(ij) \subset a} V_{ij}(x^{(ij)}) \quad .$$

2. Some ideas of the proof

We think that some of the intermediate results of the proof are almost as important as the result itself, because they allow to test our physical intuition about the quantum dynamics of N -body systems. In view of this we exempt ourselves from proving asymptotic completeness.

To each configuration of the particles one can associate a partition of these particles into clusters in such a way that particles in the same cluster are close together, and that the clusters are very distant from each other. The main intermediate result of the proof is the following statement: If at some large time t one groups the particles as explained, then the velocities of the centres of mass of these clusters are approximately given by their positions, divided by t . It is an indication that the motion of the centres of mass of these clusters is free over long times. In fact for a free particle both quantities are approximately equal. In other words, the quantum dynamics is concentrating on configurations, where these quantities coincide. A way to describe such a concentration is by use of *propagation estimates*.

Let $P(t)$ be a family of bounded, positive operators

$$P : [1, +\infty) \rightarrow \mathcal{L}(\mathcal{H}), \quad t \rightarrow P(t) \quad , \\ P(t) \geq 0 \quad .$$

A propagation estimates is an estimate of the form

$$\int_1^\infty dt (\psi_t, P(t)\psi_t) \leq \text{const} \|\psi\|^2 \quad ,$$

where $\psi_t = e^{-itH}\psi$. It tells us that the trajectory $e^{-itH}\psi$ concentrates on the region of phase-space where $P(t)$ is small.

Propagation estimates can be generated by a *propagation observable*

$$\Phi : [1, +\infty) \rightarrow \mathcal{L}(\mathcal{H}), \quad t \rightarrow \Phi(t),$$

where $\Phi(t)$ is uniformly bounded in t . We assume the existence (as a bounded operator) of the Heisenberg derivative $D\Phi(t)$, i.e.

$$\frac{d}{dt}(\psi_t, \Phi(t)\psi_t) = (\psi_t, D\Phi(t)\psi_t) \quad ,$$

which is formally given by $D\Phi(t) = i[H, \Phi(t)] + \partial\Phi/\partial t$. Assume it is positive in the sense that

$$D\Phi(t) \geq P(t) + R(t)$$

in $\mathcal{L}(\mathcal{H})$, where

$$P(t) \geq 0$$

and $R(t)$ satisfies the *remainder estimate*

$$\int_1^\infty dt |(\psi_t, R(t)\psi_t)| \leq \text{const} \|\psi\|^2 \quad .$$

Then

$$(\psi_t, \Phi(t)\psi_t)|_1^T \geq \int_1^T dt (\psi_t, P(t)\psi_t) + \int_1^T dt (\psi_t, R(t)\psi_t) \quad ,$$

where both the l.h.s. and the last term on the r.h.s. are bounded by $\text{const} \|\psi\|^2$. We conclude that $P(t)$ satisfies a propagation estimate, since the integrand is nonnegative.

We now mention two ways to prove a remainder estimate. We assume one of the following

$$1) \quad \int_1^\infty dt \|R(t)\| < \infty \quad .$$

$$2) \quad R(t) = R_1(t)^* B(t) R_2(t) + R_2(t)^* B(t)^* R_1(t) \quad ,$$

where $R_i(t)^* R_i(t)$, $i = 1, 2$ satisfy a propagation estimate and $B(t)$ is uniformly bounded. In fact

$$|(\psi_t, R(t)\psi_t)| \leq \text{const} (\psi_t, R_1(t)^* R_1(t)\psi_t)^{1/2} (\psi_t, R_2(t)^* R_2(t)\psi_t)^{1/2}$$

from which the remainder estimate follows by Cauchy's inequality.

We will now give a number of examples of propagation estimates, propagation observables, and remainder estimates. Actually they constitute the core of the proof.

Example 1. (Maximal velocity bound) Let $\Omega \subset \mathbb{R}$ be a bounded interval, and $\lambda > 0$ large enough. Then

$$\int_1^\infty \frac{dt}{t} (\psi_t, E_\Omega(H) F(\lambda \leq |x/t| \leq 2\lambda) E_\Omega(H) \psi_t) \leq \text{const} \|\psi\|^2$$

for all $\psi \in L^2(X)$, where $E_\Omega(H)$ is the spectral projection for H associated with Ω and the constant depends on Ω, λ .

The idea is that a particle with finite energy and hence speed cannot propagate into regions moving away still faster. This propagation estimate is generated by the propagation observable

$$\Phi(t) = -E_\Omega(H) h(|x/\lambda t|) E_\Omega(H),$$

where $h' \geq 0$ and $h'(y) \geq 1$ for $1 \leq y \leq 2$. One checks in fact that

$$D\Phi \geq \frac{1}{t} E_\Omega(H) F(\lambda \leq |x/t| \leq 2\lambda) E_\Omega(H) + O(t^{-2}) \quad .$$

Example 2. This example deals with free particles, $H = p^2$, and is therefore not directly applicable to N -body systems. The basic observation is that the system consisting of free particles has the classical trajectory

$$p = p_0 \quad , \quad x = 2p_0 t + x_0 \quad ,$$

where p_0, x_0 are the initial data. It follows that $(p - (x/2t))^2 = x_0^2/4t^2$ is decreasing. This suggests that one can get a positive Heisenberg derivative by considering the propagation observable

$$\Phi = -\left(p - \frac{x}{2t}\right)^2$$

(we ignore that Φ is not uniformly bounded for a while). In fact

$$D\Phi = \frac{2}{t} \left(p - \frac{x}{2t}\right)^2 \geq 0 \quad ,$$

which ‘proves’

$$\int_1^\infty \frac{dt}{t} (\psi_t, \left(p - \frac{x}{2t}\right)^2 \psi_t) \leq \text{const} \|\psi\|^2 \quad . \quad (\text{wrong})$$

This means that the time evolved quantum state is concentrating on the region in phase-space where $(p - (x/2t))^2$ is small, i.e. around the classical trajectories. But the equation above is wrong as it stands, since $\Phi(t)$ is not even a bounded operator. The next example will deal with this problem.

Example 2 (revisited). We replace Φ by a bounded operator by introducing some cutoffs, namely an energy cutoff $E_\Omega(H)$, where $\Omega \subset \mathbb{R}$ is some bounded interval, and a volume cutoff $f(x/\lambda t)$, where $f \in C_0^\infty(X)$, $f(x) = 1$ for $|x| \leq 1$, $f(x) = 0$ for $|x| \geq 2$, and $\lambda > 0$ is large. $E_\Omega f \Phi f E_\Omega$ is now a suitable propagation observable, since it is uniformly bounded in t .

$$D(E_\Omega f \Phi f E_\Omega)' = E_\Omega (f(D\Phi)f + f\Phi(Df) + (Df)\Phi f) E_\Omega \quad .$$

Since Df is supported in $\lambda \leq |x/t| \leq 2\lambda$, it is easily checked that the terms above arising from Df satisfy a remainder estimate by Example 1. Hence

$$\int_1^\infty \frac{dt}{t} (\psi_t, E_\Omega f \left(p - \frac{x}{2t}\right)^2 f E_\Omega \psi_t) \leq \text{const } \|\psi\|^2 \quad .$$

Example 3. What does Example 2 mean in the interacting case? We will give some intuition that by replacing $\left(p - (x/2t)\right)^2$ with

$$K(t) = \left(p - \frac{x}{2t}\right)^2 + V$$

we almost get the right propagation observable. Consider a configuration x . Group the particles into clusters in such a way that the particles in the same cluster are close together, and that the clusters are far from each other. Call a the resulting cluster decomposition. We express this by saying that the particles are a -clustered at x (we will be more precise about the scale which sets the meaning of far and close when introducing the partition of unity below). We split $V = V^a + I_a$, where I_a is negligible at x , i.e.

$$K(t) \cong \left(p - \frac{x}{2t}\right)_a^2 + \left(p^a - \frac{x^a}{2t}\right)^2 + V^a \quad .$$

Since the particles in the clusters of a are close together, we may try the approximation $x^a \cong 0$. Then

$$K(t) \cong \left(p - \frac{x}{2t}\right)_a^2 + H^a \quad .$$

The second term is conserved at x , and the first term is decreasing because the centers of mass of the clusters of a are free at x . Therefore $K(t)$ should have a negative Heisenberg derivative. This is however not the case, since

$$DK(t) = -\frac{2}{t} \left(p - \frac{x}{2t}\right)^2 + \frac{x}{t} \cdot \nabla V \quad ,$$

where the term arising from the potentials is not integrable in time. If the particles are a -clustered at x , then

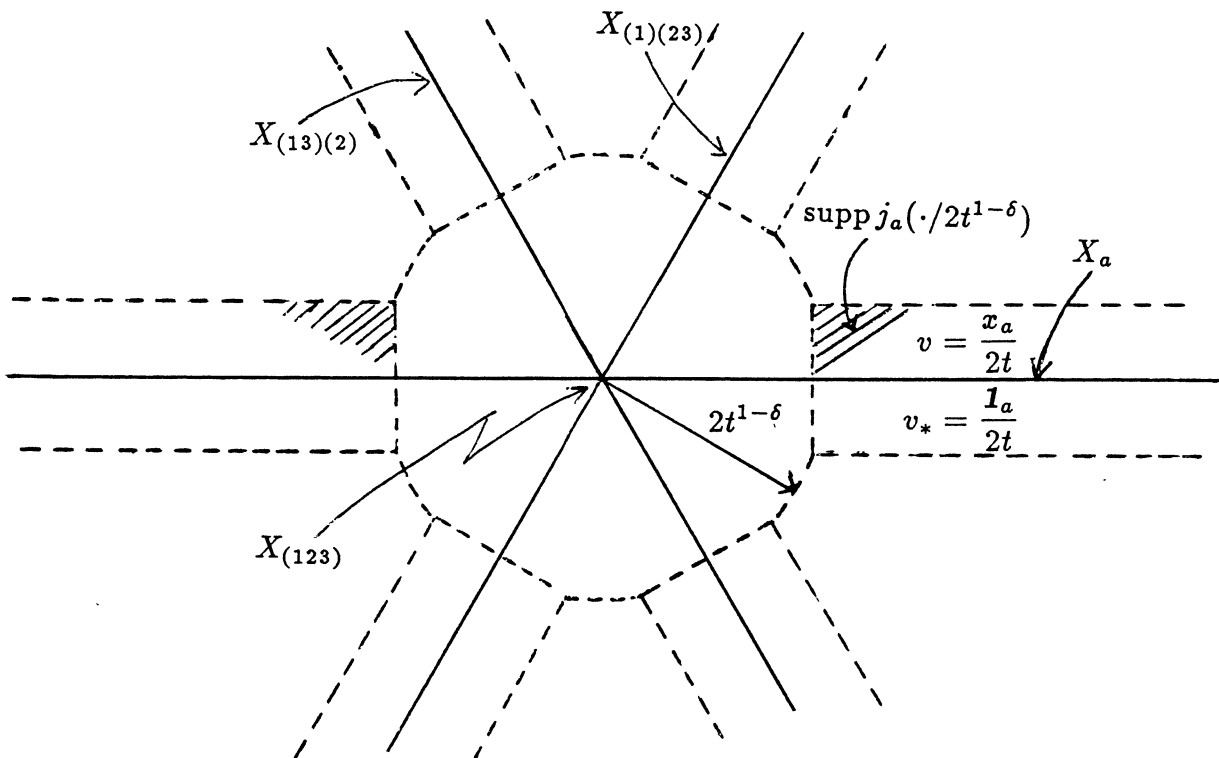
$$\frac{x}{t} \cdot \nabla V \cong \frac{x^a}{t} \cdot \nabla V^a \quad ,$$

since V^a depends on x^a alone. So we see that the approximation $x^a \cong 0$ is not allowed.

Example 3 (revisited). We replace the vector field $x/2t$ by a mild modification $v(x, t)$ of it, such that $v(x, t)^a = 0$ if the particles are a -clustered at x . More precisely we introduce a partition of unity on X

$$\sum_a j_a^2 = 1$$

which consists of smooth characteristic functions of the sets shown in the figure below. On the support of j_a the particles are a -clustered. The vector field $v(x, t)$ is then given by (a smooth version of) the one shown in the figure.



The configuration space X for $N = 3$ and the vector field v . As an example, we consider $a = (12)(3)$.

We compute

$$\begin{aligned} DK(t) = & -2(p-v)(v_* + v_*^t)(p-v) - 2\left(p \cdot \left(v_*v + \frac{1}{2} \frac{\partial v}{\partial t}\right) + \left(v_*v + \frac{1}{2} \frac{\partial v}{\partial t}\right) \cdot p\right) \\ & + 4v \cdot \left(v_*v + \frac{1}{2} \frac{\partial v}{\partial t}\right) + \Delta(\nabla \cdot v) + 2v \cdot \nabla V, \end{aligned}$$

where v_* is the x -derivative of v , and v_*^t its transpose. We evaluate these terms on each $\text{supp } j_a(\cdot/2t^{1-\delta})$ separately, disregarding the ‘boundary contributions’ arising from the fact

that v has been defined piecewise.

$$\begin{aligned}
(p-v)(v_* + v_*^t)(p-v) &= \frac{1}{t}(p-v)_a^2 = \frac{1}{t} \left(p - \frac{x}{2t}\right)_a^2, \\
\nabla I_a &= O(t^{-(1-\delta)(1+\mu_2)}) \\
v \cdot \nabla V &= \underbrace{v^a}_{=0} \cdot \nabla V^a + v \cdot \nabla I_a = O(t^{-(1-\delta)(1+\mu_2)}), \\
v_* v + \frac{1}{2} \frac{\partial v}{\partial t} &= \frac{1_a x_a}{2t} - \frac{1}{2t} \frac{x_a}{2t} = 0.
\end{aligned}$$

The results of these computations are slightly changed when making a rigorous computation with a smooth v . We mention that in this case $v_* v + \frac{1}{2} \frac{\partial v}{\partial t} = O(t^{-(1+\delta)})$, and $\Delta(\nabla \cdot v) = O(t^{-(3-2\delta)})$. As we know from the free case we have to put cutoffs around $K(t)$. Taking δ such that $\min(1+\delta, 3-2\delta, (1-\delta)(1+\mu_2)) > 1$, we get

$$D(-E_\Omega f K f E_\Omega) \geq \sum_a \frac{1}{t} E_\Omega f j_a \left(p - \frac{x}{2t}\right)_a^2 j_a f E_\Omega + \text{remainder},$$

and hence

$$\sum_a \int_1^\infty \frac{dt}{t} (\psi_t, E_\Omega f j_a \left(p - \frac{x}{2t}\right)_a^2 j_a f E_\Omega \psi_t) \leq \text{const} \|\psi\|^2.$$

For large times, this estimate asserts that whenever the particles are a -clustered, the velocities of the centres of mass of the clusters of a are approximately given by their positions, divided by t . This is the result mentioned at the beginning of this section.

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