ASYMPTOTIC COMPLETENESS OF N-BODY SCATTERING

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In my opinion, scattering theory for N-body Schrödinger operators is one of the greatest successes of 20th century mathematical physics.

On the physical side, we have a rigorous framework that explaines why nonrelativistic matter is built out of well defined clusters of nuclei and electrons, such as atoms, ions, molecules.

On the mathematical side, we have a deep analysis of a large family of nontrivial operators with continuous spectrum, combining ideas from classical and quantum mechanics.

A single quantum particle in an external potential is described by the Hilbert space $L^2(\mathbb{R}^d)$ and the Schrödinger Hamiltonian

$$H = H_0 + V(x),$$

where

$$H_0 = \frac{p^2}{2m}, \quad p = \frac{1}{\mathrm{i}}\partial_x.$$

A typical example of a potential is

$$V(x) = \frac{c}{|x|}.$$

THEOREM. Assume that $V(x)$ is short range, that is,

$$|V(x)| \leq c\langle x\rangle^{-\mu_{\mathrm{s}}}, \quad \mu_{\mathrm{s}} > 1.$$

Then there exist wave (Møller) operators

$$\Omega^{\pm} := \mathrm{s}-\lim_{t\to\pm\infty} \mathrm{e}^{\mathrm{i}tH}\mathrm{e}^{-\mathrm{i}tH_0},$$

they are isometric, they intertwine the free and full Hamiltonian:

$$\Omega^{\pm}H_0 = H\Omega^{\pm},$$

and they are complete:

$$\Omega^{\pm}\Omega^{\pm *} = 1\!\!1_{\mathrm{c}}(H).$$

THEOREM. Assume that $V(x)$ is long range, that is,

$$V(x) = V_{\mathrm{l}}(x) + V_{\mathrm{s}}(x),$$

where $V_{\mathrm{s}}(x)$ is short range and

$$|\partial_x^\alpha V_{\mathrm{l}}(x)| \leq c_\alpha \langle x \rangle^{-|\alpha|-\mu_{\mathrm{l}}}, \quad \mu_{\mathrm{l}} > 0, \ \alpha \in \mathbb{N}^d.$$

Then there exists a function $(t, \xi) \mapsto S_t(\xi)$ and modified Møller operators

$$\Omega^\pm := \mathrm{s-}\lim_{t \to \pm\infty} \mathrm{e}^{\mathrm{i}tH} \mathrm{e}^{-\mathrm{i}S_t(p)},$$

which satisfy the same properties as those stated for the short-range case.

Thus the Hilbert space is the direct sum of bound states and of scattering states – states which evolve for large times as free waves. One can define the scattering operator,

$$S := \Omega^+ \Omega^{-*},$$

which is unitary. The integral kernel of S defines scattering amplitudes. The square of the absolute value of a scattering amplitude is the scattering cross-section describing the probability of a scatteting process.

The most difficult part of the above theorems is to prove that the range of (modified) wave operators fills the whole continuous spectral space of H. This is called asymptotic completeness (AC).

2 interacting quantum particles are described by the Hilbert space $L^2(\mathbb{R}^d) \otimes L^2(\mathbb{R}^d) \simeq L^2(\mathbb{R}^{2d})$ and the Hamiltonian

$$H = \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} + V(x_1 - x_2).$$

Introduce the center-of-mass coordinate $x_{12} := \frac{m_1 x_1 + m_2 x_2}{m_1 + m_2}$ and the relative coordinate $x^{12} := x_2 - x_1$. The Hilbert space factorizes

$$L^2(\mathbb{R}^{2d}) = L^2(X_{12}) \otimes L^2(X^{12}).$$

Let $m_{12} := m_1 + m_2$ be the total mass and $m^{12} := (m_1^{-1} + m_2^{-1})^{-1}$ be the reduced mass. Then we can write

$$H = \frac{p_{12}^2}{2m_{12}} + H^{12},$$

where

$$H^{12} := \frac{(p^{12})^2}{2m^{12}} + V(x^{12}).$$

Thus the problem of two interacting particles is reduced to a single particle in an external potential.

N interacting quantum particles are described by the Hilbert space

$$\bigotimes_{i=1}^{N} L^2(\mathbb{R}^d) \simeq L^2(X),$$

where $X := \mathbb{R}^{Nd}$, and the Hamiltonian is

$$H := \sum_{j=1}^{N} \frac{p_j^2}{2m_j} + \sum_{1 \le i < j \le N} V_{ij}(x_i - x_j).$$

A typical potential is

$$V_{ij}(x_i - x_j) = \frac{Z_i Z_j e^2}{4\pi |x_i - x_j|}.$$

A cluster decomposition is a partition of $\{1, \ldots, N\}$ into clusters:

$$a = \{c_1, \ldots, c_k\}.$$

The Hamiltonian of a cluster c is

$$H_c := \sum_{j \in c} \frac{p_j^2}{2m_j} + \sum_{i,j \in c} V_{ij}(x_i - x_j).$$

The Hamiltonian of a cluster decomposition a is

$$H_a = H_{c_1} + \cdots + H_{c_k}.$$

Note that cluster decompositions have a natural order. In particular, there is a minimal cluster decompostion, where all clusters are 1-element. Every pair determines a cluster decomposition.

Define the collision plane of a as

$$X_a := \{(x_1, \dots, x_N) \in \mathbb{R}^{Nd} \ : \ (ij) \leq a \ \Rightarrow \ x_i = x_j\}.$$

Consider the quadratic form on X

$$\sum \frac{m_i}{2} x_i^2.$$

Let X^a denote the internal plane of a, defined as the orthogonal complement of X_a wrt this form. We will write $x \mapsto x_a$ and $x \mapsto x^a$ for the orthogonal projections onto X_a and X^a.

We have

$$X = X_a \oplus X^a, \quad X^a = X^{c_1} \oplus \cdots \oplus X^{c_k}.$$

Therefore,

$$L^2(X) = L^2(X_a) \otimes L^2(X^a), \quad L^2(X^a) = L^2(X^{c_1}) \otimes \cdots \otimes L^2(X^{c_k}),$$
$$\Delta = \Delta_a + \Delta^a, \qquad \Delta^a = \Delta^{c_1} + \cdots + \Delta^{c_k}.$$

For a cluster decomposition $a = \{c_1, \ldots, c_k\}$ set

$$V^a(x) = \sum_{(ij) \le a} V_{ij}(x_i - x_j) = \sum_{i,j \in c_1} V_{ij}(x_i - x_j) + \cdots + \sum_{i,j \in c_k} V_{ij}(x_i - x_j).$$

The cluster Hamiltonian decomposes:

$$H_a = \Delta_a + H^a, \quad H^a = \Delta^a + V^a(x^a),$$

$$H^a = H^{c_1} + \cdots + H^{c_k}.$$

Introduce

$$\mathcal{H}^a := \mathrm{Ran}\,\mathbb{1}_{\mathrm{p}}(H^a) \simeq \mathrm{Ran}\,\mathbb{1}_{\mathrm{p}}(H^{c_1}) \otimes \cdots \otimes \mathrm{Ran}\,\mathbb{1}_{\mathrm{p}}(H^{c_k}).$$

Let

$$E^a := H^a\Big|_{\mathcal{H}^a} = H^{c_1}\Big|_{\mathcal{H}^{c_1}} + \cdots + H^{c_k}\Big|_{\mathcal{H}^{c_k}}$$

be the operator describing the bound state energies of clusters. Let

$$J^a : L^2(X_a) \otimes \mathcal{H}^a \to L^2(X)$$

be the embedding of bound states of clusters into the full Hilbert space.

THEOREM. Assume that the potentials V_{ij} are short range. Then for any cluster decompostion a there exists the corresponding partial wave operator

$$\Omega_a^{\pm} := \mathrm{s}-\lim_{t\to\pm\infty} \mathrm{e}^{\mathrm{i}tH} J_a \mathrm{e}^{-\mathrm{i}t(\Delta_a+E^a)}.$$

$\Omega_a^{\pm}$ are isometric, they intertwine the cluster and the full Hamiltonian:

$$\Omega_a^{\pm}(\Delta_a + E^a) = H\Omega_a^{\pm}$$

and are complete:

$$\bigoplus_a \mathrm{Ran}\Omega_a^{\pm} = L^2(X).$$

THEOREM. Assume that the potentials V_{ij} are long range with

$$\mu_l > \sqrt{3} - 1.$$

Then for any cluster decompostion a there exists a function $(t, \xi_a) \mapsto S_{a,t}(\xi_a)$, the corresponding partial modified wave operator

$$\Omega_a^{\pm} := \mathrm{s-}\lim_{t \to \pm\infty} \mathrm{e}^{\mathrm{i}tH} J_a \mathrm{e}^{-\mathrm{i}(S_{a,t}(p_a) + tE^a)},$$

which satisfy the same properties as those stated in the short range case.

AC means that all states in $L^2(X)$ can be decomposed into states with a clear physical/chemical interpretation such as atoms, ions and molecules.

We can introduce partial scattering operators

$$S_{ab} := \Omega_a^{+*}\Omega_b^{-}$$

describing various processes, such as elastic and inelastic scattering, ionization, capture of an electron, chemical reactions.

The partial wave operators $\Omega_a^{\pm}$ can be organized into

$$\bigoplus_a L^2(X_a) \otimes \mathcal{H}^a \ni (\psi_a) \mapsto \sum_a \Omega_a^{\pm}\psi_a \in L^2(X),$$

which is unitary. The partial scattering operators S_{ab} arranged in the matrix $[S_{ab}]$ also describe a unitary operator.

2-body scattering theory, including AC in both short- and long-range case, was understood already in the 60's.

Existence of N-body wave operators and the orthogonality of their ranges was established about the same time. What was missing for a long time was Asymptotic Completeness – the fact that the ranges of wave operators span the whole Hilbert space.

Below I review the various methods that were used, more or less successfully, to prove this.

The stationary approach to scattering theory is based on resolvent identities. For example, if $H = H_0 + V$, then the identity

$$
\begin{aligned}
(z-H)^{-1} &= (z-H_0)^{-1} \\
&+(z-H_0)^{-1}V^{1/2}\Big(1-|V|^{1/2}(z-H_0)^{-1}V^{1/2}\Big)^{-1}|V|^{1/2}(z-H_0)^{-1}
\end{aligned}
$$

can be used to prove AC in the 2-body case.

L.Faddeev found a resolvent identity that can be used to study 3-body scattering. A number of other resolvent identities were used (eg. G.Hagedorn's for 4 bodies). The results about AC with $N \geq 3$ proven using the stationary approach involve implicit assumptions on invertibility of certain complicated operators and on properties of bound and almost-bound states. They also require a very fast decay of potentials and $d \geq 3$.

However, in principle, the stationary approach leads to explicit formulas for scattering amplitudes.

V.Enss introduced time-dependent methods into proofs of AC. In his approach an important tool was the RAGE Theorem saying that for K compact and $\psi \in \mathrm{Ran}\, \mathbb{1}^{\mathrm{c}}(H)$

$$\lim_{T\to\infty} \frac{1}{T}\int_0^T \|K\mathrm{e}^{\mathrm{i}tH}\psi\|^2 \mathrm{d}t = 0.$$

Enss started with proving the 2-body AC (late 70's), and managed to prove 3-body AC including the long-range case with $\mu_{\mathrm{l}} > \sqrt{3}-1$ (late 80's).

Let us describe an idea that turned out to be important: One needs to look for observables A such that $\mathrm{i}[H, A]$ is in some sense positive. Here is an important example of this idea:

E.Mourre (1981). Suppose that E is not a threshold (it is not an eigenvalue of H_a for any a). Then there exists an interval I around E and $c_0 > 0$ such that

$$\mathbb{1}_I(H)\mathrm{i}[H, A]\mathbb{1}_I(H) \geq c_0 \mathbb{1}_I(H),$$

where $A = \sum_i \frac{1}{2}(p_i x_i + x_i p_i)$ is the generator of dilations.

The Mourre estimate has important implications both in the stationary and time-dependent approach.

I.M.Sigal devoted a large part of his research carreer to N-body AC. After working with the stationary approach he switched to the time-dependent approach. Together with A.Soffer he obtained the first proof of the N-body AC in the short range case (announced 1985, published 1987). They first used heavily propagation estimates. Below we summarize abstractly the time-dependent version of this technique:

If $\Phi(t)$ is a uniformly bounded observable on a Hilbert space $\mathcal{H}$ and

$$\frac{\mathrm{d}}{\mathrm{d}t}\Phi(t) + \mathrm{i}[H, \Phi(t)] \geq \Psi^*(t)\Psi(t),$$

then

$$\int_1^\infty \|\Psi(t)\mathrm{e}^{-\mathrm{i}tH}v\|^2 \mathrm{d}t < \infty, \quad v \in \mathcal{H}.$$

A new and elegant proof of the N-body AC in the short range case was given by G.M.Graf (1989). Just as Sigal-Soffer's, it was also time-dependent, used propagation estimates and Mourre estimate. It introduced a clever observable, the Graf vector field, whose commutator with H is positive.

First proof of AC in the long range case for any N with $\mu_1 > \sqrt{3}-1$ (which includes the physical Coulomb potentials) was given by J.D (announced 1991, published 1993). There exists a monograph J.D and C.Gérard in Springer Tracts and Monographs in Physics, 1997[1] about this subject.

In what follows I describe the main steps of the proof. My presentation will stress some additional features of N-body scattering, which I find interesting.

[1] http://www.fuw.edu.pl/ derezins/bookn.pdf

First assume the long-range condition on the potentials with

$$\mu_{\mathrm{l}} > 0.$$

Following the ideas of the proof of Graf for the short-range case one can show the existence of the so-called asymptotic velocity:

THEOREM For any function $f \in C_{\mathrm{c}}^{\infty}(X)$ there exists limits

$$\mathrm{s-}\lim_{t \to \pm\infty} \mathrm{e}^{\mathrm{i}tH} f\left(\frac{x}{t}\right) \mathrm{e}^{-\mathrm{i}tH}. \qquad (*)$$

There exists a family of commuting self-adjoint operators $P^{\pm}$ such that $(*)$ equals $f(P^{\pm})$.

Of course, we can replace H with H^a obtaining P^{a+}, the asymptotic velocity corresponding to a. The following fact follows by arguments involving the Mourre estimate, and is also essentially due to Graf:

THEOREM For any a

$$\mathbb{1}_{\{0\}}(P^{a+}) = \mathbb{1}^{\mathrm{p}}(H^a).$$

For any a introduce

$$Z_a := X_a \backslash \bigcup_{b \not\leq a} X_b.$$

Then the family Z_a is a partition of X. In particular,

$$\mathbb{1} = \sum_a \mathbb{1}_{Z_a}(P^+).$$

Now in the short-range case AC follows easily by proving that

$$\lim_{t \to \pm\infty} \mathrm{e}^{\mathrm{i}tH_a} \mathrm{e}^{-\mathrm{i}tH} \mathbb{1}_{Z_a}(P^+)$$

exists and coincides with $\Omega_a^{\pm *}$.

In the long-range case one needs an additional step.

THEOREM Let $\phi = \mathbb{1}_{Z^a}(P^\pm)\phi$ and $\delta = \frac{2}{2+\mu}$. Then there exists c such that

$$\lim_{t\to\pm\infty} \mathbb{1}\big(t^{-\delta}|x^a| > c\big)\mathrm{e}^{\mp \mathrm{i}tH}\phi = 0.$$

To see that this bound is natural note that Newton's equation in the potential $V(x) = -|x|^{-\mu}$ at zero energy has trajectories of the form

$$x(t) = ct^{\frac{2}{2+\mu}}.$$

To prove the existence of the modified wave operator we need to show that the variation of the potential that comes from outside of the given cluster decomposition within a wave packet is integrable in time. The variation of the potential can be estimated by

$$\begin{aligned} & (\text{spread of wave packet}) \times (\text{derivative of potential}) \\ \sim \quad & t^{\frac{2}{2+\mu}} \times t^{-1-\mu}. \end{aligned}$$

The integrability condition gives

$$\frac{2}{2+\mu} - 1 - \mu < -1,$$

which is solved by $\mu > \sqrt{3} - 1$.