# Mathematical QM - Lecture 4

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## Contents

# 1 Scattering theory (part I)

Literature: Reed and Simon, Vol III: Scattering Theory; Teschl, Mathematical Methods in Quantum Mechanics.

## 1.1 Scattering is our window into the microscopic world

For example Rutherford experiment, COLTRIMS (Cold Target Recoil Ion Momentum Spectroscopy), and many more. One rare non-scattering microscopic method: Scanning tunneling microscope.

Detectors can register: direction of emission, kinetic energy of arriving particle, possibly its internal state (spin, excitation state, mass), arrival times. Arrival times are often used to determine kinetic energy from knowing time of emission and distance to the point of arrival ("time of flight" detector).

### 1.1.1 Cross section

Given an ensemble of $F_i$ incident sub-system/particles $\{\vec{k}_i, s_i, i = 1, \ldots, I\}$ with known momenta $\vec{k}_i$, internal states $s_i$ (e.g. spin, constituents, excitation state etc., if any), and flux (number of subsystems per time per surface), one measures the number per time $N_e$ of given sub-systems/particles with momenta and internal states $\{\vec{q}_e, s_e, e = 1, \ldots, E\}$. The *cross section* is the ratio

$$\sigma\left(\vec{k}_1, s_1, \ldots \vec{k}_I, s_I; \vec{q}_1, s_1, \ldots \vec{q}_E, s_E\right) = \frac{N_e}{F_i} \tag{1}$$

This is what we ultimately need to know for comparison with observation.

### 1.1.2 Potential scattering

All deeper mathematical discussion in these lectures will be limited to the case of a single particle that scatters without change of its internal state from a fixed, immutable target that is represented by a potential. I.e. $1 = I = E$ and $s_i = s_e$, such that the only relevant two arguments of the cross section are the initial and final momenta $\vec{k}_i$ and $\vec{q}_e$. Physicists call this "potential scattering".

Further we will not treat a statistical ensemble of particles but rather a particle described by a single wave function. This is a minor technical simplification useful at the present level.

## 1.2 The Lippmann-Schwinger equation

Frequently, the first form how a physics student is exposed to scattering theory is in the form of the Lippmann-Schwinger equation

$$|\Psi_{\vec{k}}^{(\pm)}\rangle = \lim_{\epsilon \downarrow 0} |\Phi\rangle - \frac{1}{H_0 - (k^2/2 \pm \imath\epsilon)} V |\Psi_{\vec{k}}^{(\pm)}\rangle. \tag{2}$$

This is an equation for "scattering eigenfunctions" (in/out)

$$H|\Psi_{\vec{k}}^{(\pm)}\rangle = \frac{k^2}{2}|\Psi_{\vec{k}}^{(\pm)}\rangle \tag{3}$$

with the Hamiltonian

$$H = H_0 + V \tag{4}$$

$H_0$ the "free" Hamiltonian, $V = H - H_0$ the interaction (potential), and $\Phi\ldots$ "scattering eigenfunction" of $H_0$

$$H_0\Phi = E\Phi \tag{5}$$

Usual choice

$$H_0 = -\frac{1}{2}\Delta \quad (\textbf{or} : -\Delta) \tag{6}$$

The quotation marks indicate that the "eigenfunctions" are not in the Hilbert space and therefor their existence and meaning need to be related to the operators that are defined as linear operators in Hilbert space.

In position space the Lippmann-Schwinger equation is an integral equation

$$\Psi^{(\pm)}(\vec{r}) = e^{\imath\vec{k}\cdot\vec{r}} - \frac{1}{4\pi}\int d^{(3)}r' \frac{e^{\mp\imath|k||\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|}V(\vec{r}')\Psi^{(\pm)}(\vec{r}') \tag{7}$$

It is not at all obvious how this equation is related to the above description of a scattering experiment. How, for example, would we extract a cross section from $\Psi^{(\pm)}$? And why would it be related to the time-dependent definition of scattering given above? And how do $\Psi^{(\pm)}$ fit into our Hilbert space formulation of quantum mechanics? Later in this introduction we will by formal manipulations derive the equation. Historically, of course, it derives from the well studied scattering of classical waves. Here, for the conceptually clear definition of scattering theory we use the limit of standard time-dependent quantum mechanics to large times, as one does effectively in an experiment, where detection occurs at macroscopically large times and at macroscopically large distances after a microscopic scale reaction.

### 1.3 Mathematical modeling of a (simple) scattering experiment

Prepare a particle in some "free" state, e.g. free wave packet

$$\Phi(\vec{r}, -t) = (2\pi)^{-3/2}\int d^{(3)}k e^{i\vec{k}\cdot\vec{r}}\psi(\vec{k}) \tag{8}$$

at some time $-t$. Prepare the packet such that no part of it is in the range of interaction.

Let that wave packet evolve *according to the scattering time-evolution.* Wait long enough, say, until $t$, and analyze the wave packet outside the range of the interaction.

The fundamental mathematical issues are:

- What does "preparing the state" mean? Can we actually map any arbitrary free wave packet into a scattering wave packet? Is that mapping unique? (**Existence and uniqueness** of scattering solutions.)

- What is the fate of the scattering state? Can the system just "swallow" an incoming particle? Or can we be certain to find the system again in a (possibly quite different) free wave packet at some large time $t$? (**"Asymptotic completeness"**)

### 1.4 Point spectrum, absolutely continuous spectrum, and others

A brief reminder: spectral subspaces

$$\mathcal{H}_p = \overline{\text{span}(eigenvectors)} \tag{9}$$

and

$$\mathcal{H}_c = \mathcal{H}_p^{\perp} \tag{10}$$

The continuous spectrum consists of the singular continuous spectrum *sc* and absolute continuous *ac* spectrum and the complete space is

$$\mathcal{H} = \mathcal{H}_p \oplus \mathcal{H}_{ac} \oplus \mathcal{H}_{sc} \tag{11}$$

Functions $\psi \in \mathcal{H}_{ac}$ behave like wave packets, i.e.

$$\lim_{t \to \pm\infty} \langle e^{-itH}\psi | \psi \rangle = 0, \tag{12}$$

we can say: after long time, the wave packet becomes orthogonal to its original.

For functions from the *sc* spectrum a similar decay only holds in the time-averaged sense. This kind of spectrum is poorly suitable for scattering considerations, as we cannot exclude that the system returns to its initial state, even if only for a short time. Note that Hamiltonians with *sc* spectrum are not necessarily pathological cases: they may possibly be realized in quasi-crystals (i.e. with quasi-periodic potentials). We will not consider them for our discussion of scattering theory.

### 1.5 Relatively compact and relatively bounded operators

Scattering is cast into a mathematical concept by comparing a known (usually the free) time-evolution with generator $H_0$ two an unknown evolution for $H$. For this comparison to work the difference between the evolutions $V = H - H_0$ should be "not too big". Two useful definitions for comparing two operators:

**Definition 1.** *Let $A$ be self-adjoint and $D(B) \supseteq D(A)$, the we call $B$* **relatively compact** *to $A$, if $B(H - z)^{-1}$ is compact, we call it* **relatively bounded**, *if $B(H - z)^{-1}$ is bounded.*

**Compact operators:** Remember that compact can be understood as "well approximated by finite-rank operators", i.e. a compact operator's action differs from $\epsilon$ only on a finite subspace. "Relatively compact" could be understood as follows: comparing the operator $C$ to $H$, one finds that except on a finite subspace, $C$ is smaller than $H$ by any desired factor $\epsilon$. Remember also that compact operators have the nice property of turning weakly convergent sequences into strongly convergent sequences. The reason why this happens is intuitively clear: typically, a weakly convergent sequence consists of vectors

that do not really settle in onto a single vector, but keep turning into new directions of the infinitely dimensional space. A compact operator reduces all but a few of those ever new additions to length $\epsilon$.

Relative compactness means that the significant (i.e. $> \epsilon$) differences between the operators are limited to a finite subspace. Relative boundedness is an important property in perturbation theory, as it allows to consider one operator as "small" compared to the other.

## 1.6 Mapping between free and scattering states — scattering operators $\Omega_\pm$

The key objects of scattering theory are the "scattering operators" $\Omega_\pm$ that map between the two time-evolutions. Existence and asymptotic completeness of scattering theory is formulated in terms of the $\Omega_\pm$.

Go far back in time such that the particle is almost certainly outside a preset finite volume. We expect this behavior as a result of wave packet broadening. This intuition is made precise and proven in the form of the **RAGE theorem**. It establishes a relation between the different spectra types and the long-time behavior of a wave packet. One can paraphrase this theorem as follows: for any wave packet in the *absolutely continuous* spectrum $\psi \in \mathcal{H}_{ac}$ of some operator $H$ and any operator $C$ that is bounded and not too big compared to $H$, the time-average

$$\frac{1}{T}\int_{-T}^{T} ||Ce^{-iHt}\psi||^2 \overset{T\to\infty}{\to} 0 \tag{13}$$

goes to zero. "Not too big" is specified as $C(H+i)^{-1}$ being a compact operator. This property is rather important in various contexts and sometimes is given the name "relatively compact". Similarly, RAGE also says that wave packets composed of states from the *point spectrum* remain located in a finite region of space.

### 1.6.1 Long-term time-evolution for continuous spectrum

Relative compactness allows us to single out a "finite" subspace in the spectral range of an operator. The following theorem tells us, that no wave packet from the continuous spectrum can ever be contained in such a finite subspace in the long run.

**Theorem 1.** *Let $A$ be self-adjoint and $K$ be relatively compact and denote by $P^{(c)}\mathcal{H} = \mathcal{H}_c$ and $P^{(ac)}\mathcal{H} = \mathcal{H}_{ac}$ the projectors onto the continuous and absolutely continuous spectra, respectively, then*

$$\lim_{T\to\infty}\frac{1}{T}\int_0^T ||Ke^{-iAt}P^{(c)}\psi||^2 dt = 0, \qquad \lim_{T\to\infty}||Ke^{-iAt}P^{(ac)}\psi||^2 = 0$$

*for every $\psi \in \mathcal{D}(A)$. If in addition $K$ is bounded, then the result holds for every $\psi \in \mathcal{H}$.*

### 1.6.2 Implication for Schrödinger operators

One finds that the characteristic function $C$ of any finite sphere is relatively compact to the free motion Hamiltonian $-\Delta$, i.e. any free wave packet goes to arbitrarily far spatial

distances eventually. If also the interaction decays sufficiently fast, then the time-evolution will be indistinguishable from a free time-evolution.

**Remark on the Coulomb potential:** Unfortunately, the long range tail of the Coulomb is does not decay "sufficiently fast". For the Coulomb potential, the mathematical proofs given in the lecture do not work. In fact, the scattering theory into free states does not exist. There is a comparatively cheap way out of this problem, which will be discussed later.

#### 1.6.3 The RAGE theorem

The RAGE theorem sharpens the above in the sense that point- and continuous spectrum of any self-adjoint operator $A$ are fully characterized by the long-time behaviour of the dynamics $A$.

**Theorem 2.** *(RAGE). Let $A$ be self-adjoint. Suppose there is a sequence of relatively compact operators $K_n$ which converges strongly to identity. Then*

$$\mathcal{H}_c = \{\psi \in \mathcal{H} | \lim_{n\to\infty} \lim_{T\to\infty} \int_0^T ||K_n e^{-itA}\psi|| dt = 0\}$$
$$\mathcal{H}_p = \{\psi \in \mathcal{H} | \lim_{n\to\infty} \sup_{t\geq 0} ||(\mathbf{1} - K_n)e^{-itA}\psi|| dt = 0\}$$

This theorem tells us that we can characterize $\mathcal{H}_c$ and $\mathcal{H}_p$ completely by the behavior of functions under the long-time limit of quantum mechanical evolution: the first part says that the fact that wave packets composed of the continuous spectrum will be "diluted" out of any "finite" subspace. "Finite" means the space where $K$ differs relevantly from $A$ (relatively compact). In physics terms: if a wave packet fully spreads (in the time-average), then it completely belongs to the continuous spectrum.

The second part tells us that if we can find a "finite" space (in the sense as above) where the wave-packet remains contained, the wave packet belongs purely to the continuous spectrum: spectral properties and time-evolution behavior match one-to-one.

#### 1.6.4 Existence of the $\Omega_\pm$

Assume that far back in time a given wave packet can escape the action of the potential. At that time, free and interacting time evolution are indistinguishable for the wave packet. We may then consider the wave packet as an interacting one and evolve forward in time to the present by the full time evolution. Under which circumstances can we find times large enough to do such a mapping? Do the following limits exist:

$$\lim_{t\to\pm\infty} U(t)U_0(-t) := \Omega_\pm? \tag{14}$$

In which sense may the limits exist? Can it exist in an operator sense? Given $\epsilon$,

$$?\exists T : ||U(t)U_0(-t) - \Omega_\pm|| < \epsilon, \quad \forall t > T \tag{15}$$

("Uniformly" for all states): probably not, we only need to choose arbitrarily slow wave packets, i.e. particles that move extremely slowly out of the interaction region at a speed

$v < L/T$, where $L$ is some characteristic dimension of the interaction region. However, it may exists "pointwise" for any wave packet

$$||[U(t)U_0(-t) - \Omega_\pm]|\Phi\rangle|| \to 0. \tag{16}$$

That is, the time-limit can exist in the sense of a *strong limit*.

#### 1.6.5 Asymptotic completeness

At finite times $t$ the operator $U(t)U_0(-t)$ is unitary. Can the limits $\Omega_\pm$ be unitary? Hardly, we know that bound states (any vector from the point-spectrum) cannot appear in the range of $\Omega_\pm$ (those states, according to RAGE, would never get out of some finite range).

Although the $\Omega_\pm$ will not be unitary in general, they can still be bijections. We would like them to be bijections between the space of all free states, i.e. all wave packets formed in $P_{ac}(H_0)\mathcal{H}$ and all scattering states, which we define as wave packets from $P_{ac}(H)\mathcal{H}$. Note that for $H_0 = -\Delta$: $P_{ac}\mathcal{H} = \mathcal{H}$. If the $\Omega_\pm$ are such bijections, we say that scattering is **asymptotically complete**.

The physical meaning of asymptotic completeness is that scattering states and localized states do not mix: localized remains localized, scattering remains scattering. It just does not happen, that a wave packet goes in and turns into a bound state or gets stuck in some other way. All that goes in comes out again. Neither does it happen that a localized state decides to decay. Of course, in physics such processes do seem to occur, they go by the name of "capture" or "decay" or so: looking more closely, in these processes either another constituent goes out (e.g. a photon is emitted) or some long-lived intermediate state is formed (a resonance), that will decay eventually.

As often, an example where the scattering operators exist, but are not asymptotically complete is interesting, (see Reed and Simon III, counterexample to Theorem XI.32, p.70).

#### 1.6.6 Scattering operators as unitary maps $P_{ac}(H_0)\mathcal{H} \to P_{ac}(H)\mathcal{H}$

The scattering operators map the unbound dynamics of $H_0$ and $H$ onto each other in the sense that $\chi \in P_{ac}(H_0)\mathcal{H}$ and $\Omega_\pm\chi = \psi \in P_{ac}(H)\mathcal{H}$ have the time evolutions

$$\Omega_\pm e^{-itH_0}\chi = e^{-itH}\psi = e^{-itH}\Omega_\pm\chi \tag{17}$$

So, commuting any exponential through the scattering operators replaces $H$ with $H_0$. For exponentials, this is easy to show. By Fourier transform it carries over to all bounded functions of $F$ and goes by the name of "intertwining":

$$f(H)\Omega_\pm = \Omega_\pm f(H_0). \tag{18}$$

Note that as strong limits of unitary operators the $\Omega_\pm$ will conserve the norm, i.e. they will be isometries. If they also map the complete subspaces onto each other, they will be unitary operators. Therefore, asymptotically complete scattering operators are unitary maps between the *ac* spectral spaces of $H_0$ and $H$.

### 1.6.7 Scattering operators compare two dynamics

We see that the roles of $H_0$ and $H$ enter symmetrically: the scattering operators connect two unitarily equivalent dynamical systems. Scattering theory compares one known dynamics to another one, maybe less well known. From a mathematical point of view, it is irrelevant, which is which. Physically, of course, we know everything about, say, $-\Delta$ and often rather little about $-\Delta + V$.

But, for example, we know also a lot about the Coulomb problem (all eigenfunctions and generalized scattering eigenfunctions) and we could just as well use the Coulomb Hamiltonian as our $H_0 = -\Delta - 1/r$ and compare another dynamics, that only asymptotically behaves Coulomb-like. Of course, the *ac* "eigenfunctions" of $-\Delta$ are just plane waves, which are much easier to handle than the hypergeometric scattering functions of the Coulomb problem.

Unbound Coulomb dynamics itself is *not* unitarily equivalent to free motion. We will need to construct a different dynamics to establish such an equivalence (Dollard Hamiltonian).