Mathematical QM - Lecture 5

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Contents

1 Scattering theory (part II)

1.1 Asymptotic completeness - guide through the proof by Enss

A rather elegant proof of asymptotic completeness for an important class of Hamiltonians was given by Volker Enss [Comm. Math. Phys. 61, 285, (1978)]. Here we provide a sketch of the proof, mostly in the form of comments to the version of the proof given in Teschl, Mathematical Methods in Quantum Mechanics.

Watch out: recent mathematical physics uses different sign conventions for the scattering operators than physicists. The rift in sign conventions goes right between Reed and Simon, and, for example, Teschl. We use the modern convention.

1.1.1 Short range potentials

The discussion is restricted to $H_0 = -\Delta$ and $H = H_0 + V$. First requirement is that the potential V be "relatively bounded" to $-\Delta$, i.e. $||V(-\Delta + 1)^{-1}|| < \infty$.

A relatively bounded perturbation V of the Laplacian $-\Delta$ is called *short range* if

$$\int_0^\infty ||V(-\Delta + 1)^{-1}\mathbf{1}_{\mathbb{R}^3 \setminus B_r}||dr < \infty \tag{1}$$

where $B_r := \{x \in \mathbb{R}^3, |x| < r\}$. Relative boundedness guarantees that the integrand is always finite. This is not as strong a constraint as it may seem: for example, also the Coulomb potential is relatively bounded to $-\Delta$. What matters is that the remote parts of the potential drop sufficiently fast compared to the kinetic energy. That this is *not* the case for the Coulomb potential.

Technically, the short range property is mostly exploited in the form of the compactness of

$$(H - z)^{-1} - (H_0 - z)^{-1} \quad \text{and} \quad f(H) - f(H_0) \tag{2}$$

The existence of the scattering operators is guaranteed by **Cook's criterion**: If

$$\int_{t_0}^\infty dt||Ve^{\pm itH_0}\phi|| < \infty \tag{3}$$

for all functions ϕ from a dense subset of $P_{ac}(H_0)\mathcal{H}$, then the scattering operators exist. This follows relatively easily directly from the definition of the scattering operators (sorry for skipping domain specification).

1.1.2 Exclusion of the *sc* spectrum

Asymptotic completeness requires some reasoning in terms of spectral theory to exclude complications with the singular continuous spectrum. Here we are helped by the fact that we "know" that $-\Delta$ has purely *ac* spectrum. If perturbations are added that are not too wild, we will only generate a few bound states, maybe resonances, but no spectrum of *sc* character. However, we skip this discussion here and assume there is no *sc* spectrum.

1.1.3 Idea of the proof

The idea of Enss proof is clearly spelled out in his original paper: take any wave packet $\psi \in P_{ac}(H)$ to a remote time in the future $e^{-itH}\psi = \psi(t)$. At that time, decompose it into parts that go out, i.e. parts where position vector and momentum point to the same direction from the scattering potential (assumed to be located near the origin) $\vec{x} \cdot \vec{p} > 0$, and parts that go in $\vec{x} \cdot \vec{p} < 0$.

As a first step, this decomposition can be used to show that the scattering operators exist via Cook's criterion. Once we know the scattering operators exist, we also know that

$$\Omega_{\pm} P_{ac}(H_0)\mathcal{H} \subset P_{ac}(H)\mathcal{H} \tag{4}$$

As asymptotic completeness is equivalent to

$$\Omega_{\pm} P_{ac}(H_0)\mathcal{H} = P_{ac}\mathcal{H}, \tag{5}$$

one only needs to show

$$\Omega_{\pm} P_{ac}(H_0)\mathcal{H} \supset P_{ac}\mathcal{H}, \tag{6}$$

i.e. any scattering wave packet $\psi \in P_{ac}(H)\mathcal{H}$ is also $\psi \in \Omega_{\pm} P_{ac}(H_0)\mathcal{H}$. This second and decisive step is made as follows: at large positive times t, outgoing components cannot interact in the future, as they will never get near to the potential, from which one concludes that outgoing components remain in $\operatorname{ran}\Omega_+$. Ingoing components, on the other hand, at sufficiently large positive times, *due to the particular short range nature* of the potential, are essentially restricted to a finite-dimensional space. As the scattering wave-packet converges weakly to 0, at large times it will become orthogonal to the near finite-dimensional ingoing components. From this one can conclude that the outgoing wave-packet is $\phi(t \to \infty) \in \operatorname{ran}\Omega_+$. One remembers that $\operatorname{ran}\Omega_\pm$ is invariant under the time-evolution, so if ever $\phi(t) \in \operatorname{ran}\Omega_\pm$ for any time, it stays there for all times. The time-limit $t \to -\infty$ shows $\phi(t) \in \operatorname{ran}\Omega_-$.

For the reasoning to work one needs to be able to neglect the potential at one point compared to the kinetic energy parts of the operator, otherwise the identity of "ingoing" and "outgoing" cannot be established with sufficient accuracy. This is what restricts the proof (and the present formulation of scattering theory as a whole), to *short range potentials* (see above and Teschl Eqs. (12.29) and (12.30)).

1.1.4 In- and outgoing spaces

But how to decompose the wave packet into some kind of in- and out parts without resorting to the scattering operators themselves? The division into in- and outgoing parts of the ψ is achieved by constructing $\vec{x} \cdot \vec{p}$ as a self-adjoint operator projecting onto the positive and negative spectral subspaces. $D = \frac{1}{2}(\vec{x} \cdot \vec{p} + \vec{p} \cdot \vec{x})$, the self-adjoint generator of the (unitary) dilation group

$$U_\lambda \Psi(\vec{x}) = (e^\lambda)^{3/2} \Psi(e^\lambda \vec{x}), \quad U_\lambda =: e^{ie^\lambda D} \tag{7}$$

By Stone theorem, the generator D of a differentiable, one-parameter unitary group (U_λ) is selfadjoint (Teschl (10.9) and (12.18)). Spectral projectors are used to split the space into parts with positive (out) and negative (in) dilation rate, i.e. $P_\pm := P_D((0, \pm\infty))$.

1.1.5 Escape of the wave packet - Perry's estimate

Just how successfully the wave-packet escapes the influence of the potential is quantified by Perry's estimate (Teschl, Lemma 12.5). To specify this, one needs to battle a few technical complications: first of all, very slow particles escape the potential very slowly. For any estimate, we need to have a least an ϵ of velocity. For any ϵ we can formulate a sufficiently strong estimate. This still provides a dense set of functions to work with. Secondly, one has a similar problem with the division into in and out: when particles are very close to the origin or spiral very slowly away from the origin, the distinction may not be sharp enough, although velocities may be high. Again, we need to make the estimate starting from some finite dilation rate R by using the projector $P_D((\pm R, \pm\infty))$ rather than $P_\pm = P_D((0, \pm\infty))$. Perry's estimate then is

$$||1_{B_{2v|t|}} e^{-itH_0} f(H_0) P_D((\pm R, \pm\infty))|| \leq \frac{C}{1+|t|^N} \quad \text{for} \quad \pm t > 0. \tag{8}$$

for any N. R here indicates just how much of the total space we exclude from the estimate. This can be arbitrarily little, i.e. the estimate can be realized for a dense subset. The function $f(H_0) : \text{supp}\, f \subset [v_0^2, v_1^2]$ restricts the kinetic energies that are taken into account to a finite, but arbitrary range excluding zero. v of $B_{2v|t|}$ is smaller than v_0, i.e. the sphere on which we look for particles grows more slowly that how the particles leave. We see, the probability of a particle being inside the slowly growing sphere drops faster than any inverse power of $|t|$.

Note that the functions of the form

$$\psi = f(H_0) P_D((\pm R, \pm\infty))\varphi \tag{9}$$

are dense in the Hilbert space.

1.1.6 Existence of scattering operators by Cook's criterion

The existence of scattering operators is shown by Cook's criterion, where the boundedness of the integrals is shown by splitting the integral into an inner region and an outer region with a time-dependent radius separating the two regions. In the outer region, it is finite because of the short range assumption. In the inner region Perry's estimate can be administered for a dense set of functions of the form where both spectral constraints discussed above are applied (Teschl 12.32). Somewhat loosely speaking: scattering operators exists because the interacting wave packet leaves from near the potential sufficiently rapidly (Perry estimate) and at larger distances not much happens (short range).

Note that we originally have formulated the Perry estimate only for free motion, but relative boundedness of the potential ensures that there is no substantial difference between interacting and free motion.

1.1.7 Compactness — in- and outgoing parts are almost free wave packets

Teschl Lemma 12.10 is essential for the whole idea of the prove. Stating that $(\Omega_\pm - \mathbf{1}) f(H_0) P_\pm$ is compact shows that classifying the components as in- or outgoing by their

behavior under dilatations is meaningful: on the separate pieces, the scattering operators differ "little" from **1** (again with the precaution of not including too small velocities by applying $f(H_0)$). "Little" here means by less than ϵ except on a finite dimensional subspace.

1.1.8 Final steps of the proof

What is left to show is that any scattering wave packet is $\psi \in \mathrm{ran}\Omega_+$ and $\psi \in \mathrm{ran}\Omega_-$. Both signs are shown by the same procedure, we discuss only Ω_+. We will do this by showing that any scattering wave packet $\psi_\perp \ni \mathrm{ran}\Omega_+$ has $||\psi_\perp|| = 0$

(12.38): The first observation is that any wave packet with finite velocity ultimately decomposes into in- and out-packets as $t \to +\infty$:

$$e^{-itH}\psi =: \psi(t) \sim \varphi_-(t) + \varphi_+(t), \quad \varphi_\pm(t) \in P_\pm \mathcal{H} \tag{10}$$

Here short range and ensuing compactness of differences between functions of $f(H)$ and $f(H_0)$ is essential.

(12.40): At sufficiently large times, we can apply the scattering operators to the in- respectively out-packets without substantially changing them

$$\varphi_\pm(t) \sim \Omega_\pm \varphi_\pm(t). \tag{11}$$

(12.41): This is used to show that asymptotically the norm of any wave packet can be expressed by using the time-limits involving the in- and out-packets:

$$||\psi||^2 = \lim_{t\to\pm\infty} \langle \psi(t) | \Omega_+\phi_+(t) + \Omega_-\phi_-(t)\rangle \tag{12}$$

(12.42): If we assume that there is a scattering wave packet $\psi_\perp$ orthogonal to $\mathrm{ran}\Omega_+$. Only the in-packet $\Omega_-\phi_-(t)$ can contribute to the norm $||\psi_\perp||$.

(12.43): However, as for $t \to +\infty$ also that contribution is zero, we know that there is no scattering wave packet orthogonal to $\mathrm{ran}\Omega_+$. In this final step one uses the plausible Corollary 12.6, saying that at large positive times one finds hardly any ingoing parts in any wave function evolving under the free time-evolution:

$$P_D((-R,-\infty))f(H_0)\exp(-itH_0) \to 0 \quad \text{for} \quad t \to +\infty \tag{13}$$

With the corresponding sign changes one proves that there is also no scattering wave packet orthogonal to $\mathrm{ran}\Omega_-$ and asymptotic completeness is proven.

2 Coulomb scattering

[Reed and Simon, section XI.9]

The wave-operators for $H = -\Delta - 1/r$ and $H_0 = -\Delta$ do not exist

$$w - \lim_{t\pm\infty} e^{it(-\Delta - 1/r)} e^{-it(-\Delta)} = 0 \tag{14}$$

Why? Classical scattering: the hyperbolas of the classical 1/r potential *do* approach straight lines sufficiently well. However, any particle on a Coulomb hyperbola will outrun any free particle with the same asymptotic energy, no matter how far away from the force-center one starts, specifically with the time-dependence

$$r(t) = ct + d\log t + O(1). \tag{15}$$

While the linear time-dependence is exactly what we expect for free motion, the logarithmic dependence causes trouble: assume that at one point T_0 in time free and Coulomb positions are close. Then a there is always a later time T_1 when the two positions differ by an arbitrary distance L. This, in the end, is also the reason for the weak convergence $\to 0$ of the quantum scattering operators.

How to repair? Choose a different comparison time-evolution! Do not compare to a free particle, but to something that gets accelerated just enough to keep up with the Coulomb particle. Define Dollard wave operators with the time-dependent Hamiltonian

$$H_D(t) = -\Delta - \frac{1}{2|t|\sqrt{-\Delta}}\theta(-4|t|\Delta - 1) \tag{16}$$

and it turns out

$$\Omega_{\pm}^{(D)} = s - \lim_{t\to\pm} e^{it(-\Delta - 1/r)} e^{-i\int_0^t H_D(s)ds} \tag{17}$$

exists. Again Volker Enss (1979) proved asymptotic completeness for Dollard comparison operators (not in the 1972 Reed and Simon book).

Apart from the technical complications, does H_D define useful dynamics for the comparison? It turns out yes, as momentum information that we are interested in is unaltered. The long time limit of momenta is the same as for free motion, this is what is usually measured. What changes is the exact interpretation of arrival times at the detector, but that is usually not considered. Actually, it is hard to observe as in a typical scattering experiment there is no information on when exactly the interaction takes place, and therefore how long time the particle traveled before it hit the detector. (Note the arrival times can be measured very accurately.)

2.1 Exact solutions

Like in the classical case, we also know the exact scattering solutions of the quantum Coulomb problem. And we know the mapping of incoming to outgoing asymptotic momenta. In that sense the single particle Coulomb scattering problem can be considered as solved.

The reason for this solvability is the same as in the classical case: high symmetry of the system. Except for angular momentum and energy, there is one more conserved vector: the Lenz-Runge vector: the "perihelium" position in classical mechanics.

It turns out that "asymptotic momentum operators" $p_\pm$ can be defined (compare the classical hyperbolas), in terms of which $HP_{ac} = p_\pm^2$. After that, the scattering problem can be solved with purely algebraic methods (for details, see Thirring).

2.2 Coulomb + finite range potentials

As the Coulomb dynamics is known completely, we can use it instead of the free motion as a comparison time evolution for dynamics, that are long range Coulomb but have short range modifications. Think of the scattering from the ion of a molecule.

Suppose we have a Hamiltonian of the form

$$H = -\Delta - 1/r + V = H_c + V \tag{18}$$

where $V(H_c - i)^{-1}$ is bounded and short range. Then the same apparatus of scattering theory can be run for the wave operators

$$\Omega_{\pm}^{(c)} = \lim_{t \to \pm\infty} e^{itH} e^{-itH_c} \tag{19}$$

which will map $\mathcal{H}(H_c)_{ac} \to \mathcal{H}(H)_{ac}$. Existence of the scattering operators is proven (e.g. Muleherin and Zinnes, 1970). Asymptotic completeness $\mathrm{ran}\Omega_{\pm}^{(c)} = \mathcal{H}(H)_{ac}$, can be inferred from the result of Enss the general asymptotic completeness for long-range ($\sim 1/r$) potentials relative to Dollard operators.

3 Formal derivations

In this section we do not even try to give rigorous results. Rather, we show a few manipulations that relate the rigorous results of the previous section to what physicists often do.

3.1 The Lippmann-Schwinger equation in disguise

The LS equation is of great practical importance in physics. We introduced it as an equation for the "scattering eigenfunctions" $H\Psi_{\vec{k}}^{(\pm)} = \frac{k^2}{2}\Psi_{\vec{k}}^{(\pm)}$. Unfortunately, rigorous foundation of "scattering eigenfunctions" and derivation of related formulae of practical importance requires the buildup of a significant mathematical apparatus. Here we will introduce the "dirty" physicist's formal manipulations that lead from the scattering operators to the LS equation and further on to cross-sections.

Take an arbitrarily narrow free wave packet "$\varphi_{\vec{k}} \sim e^{i\vec{k}\cdot\vec{r}}$", then

$$|\Psi^{(\pm)}\rangle := \Omega_{\pm}|\varphi_{\vec{k}}\rangle \tag{20}$$

is indeed a seemingly much simpler equation than the LS equation to obtain scattering states $\Psi^{(\pm)}$. The $\Psi^{(-)}$ is what we want as an "in" state: in the far past it looks like the free wave packet $\psi_{\vec{k}}$. The similarity becomes even more evocative, when we will show that in the spectral representation of H_0 we have

$$\Omega_{\pm} = 1 - \lim_{\epsilon \downarrow 0} \int_0^{\infty} (H - E \pm i\epsilon)^{-1} V \delta(H_0 - E) dE \tag{21}$$

We use the notation for the spectral measure $dP(E) = \delta(H_0 - E)dE$ (we have a pure ac spectrum and therefor no trouble with possible point spectrum. Some signs need

adjustment, but most importantly we have the resolvent of H, not H_0. Unfortunately, this makes this formula useless for computations. But it can be transformed to the LS equation.

Sign convention We use here the sign convention that the $\Psi^{(\pm)}$ carry the same sign as the wave operators $\Omega_\pm$. It also appears natural to associate the limit through the remote past with the $-$, remote future with $+$. Be warned that traditional physics literatur often uses different conventions, where the sign reflects from which side in the complex plane the real energy axis is approached.

3.2 $\Omega_\pm$ in the spectral representation of H_0

$\Omega_\pm$ are time-independent operators operators obtained as time limits of time-dependent operators. Here we will replace the limit in time by a limit of resolvents of H_0. This is achieved by using a result by Abel:

Let f be a bounded function on $(0,\infty)$ and suppose $\lim_{t\to\infty} f(t) = f_\infty$. Then

$$\lim_{\epsilon\downarrow 0} \epsilon \int_0^\infty e^{-\epsilon t} f(t) dt = \lim_{t\to\infty} f(t). \tag{22}$$

Problem 3.1: Abel limit Show that

$$V(t) \to V_\infty \qquad \Rightarrow \qquad \lim_{\epsilon\downarrow 0} \epsilon \int_0^\infty e^{-t\epsilon} V(t) dt = V_\infty$$

as a strong limit. In the same way we can evaluate the limits of $e^{itH}e^{-itH_0}$, where we heavily rely on the intuition that we can treat operators just like numbers as long as we respect their non-commuting nature (and take care of domain questions).

Derivation In the spectral representation of H_0

$$H_0 = \int_0^\infty E dP(E) \tag{23}$$

we write

$$e^{itH}e^{-itH_0} = e^{itH}\int_0^\infty e^{-itE} dP(E) = \int_0^\infty e^{it(H-E)} dP(E) \tag{24}$$

The integrals exists, as the involved functions and operators are bounded. Now we use the Abel method and formally the time-integral

$$\begin{aligned}
\Omega_\pm &= \lim_{\epsilon\downarrow 0} \epsilon \int_0^\infty e^{-\epsilon t} \int_0^\infty e^{\pm it(H-E)} dP(E) dt && (25)\\
&= \lim_{\epsilon\downarrow 0} \epsilon \int_0^\infty \int_0^\infty e^{\pm it(H-E\pm i\epsilon)} dt\, dP(E) && (26)\\
&= \lim_{\epsilon\downarrow 0} \pm i\epsilon \int_0^\infty (H-E\pm i\epsilon)^{-1} dP(E) && (27)\\
&= 1 - \lim_{\epsilon\downarrow 0} \int_0^\infty (H-E\pm i\epsilon)^{-1} V dP(E) && (28)
\end{aligned}$$

The last step is by some algebra with the resolvent

$$\begin{aligned}
(H-E\pm i\epsilon)^{-1}(\pm i\epsilon) &= (H-E\pm i\epsilon)^{-1}[(H-E\pm i\epsilon) - (H-E)] \\
&= 1 - (H-E\pm i\epsilon)^{-1}(H_0+V-E) && (29)
\end{aligned}$$

and observing that

$$(H_0-E)dP(E) = (H_0-E)\delta(H_0-E)dE = 0.$$

For the time integral we have treated H like an ordinary function: as it is selfadjoint, it has a spectral representation

$$H = \int G dP_H(G) \tag{30}$$

for the projection valued measure P_H belonging to H. Then

$$\int_0^\infty e^{\pm it(H-E\pm i\epsilon)} dt = \int \int_0^\infty e^{\pm it(G-E\pm i\epsilon)} dP(G) dt \tag{31}$$

with $G \in \sigma(H) \subset \mathbb{R}$. Integrals can be interchanged, the time integral can be performed and the spectral representation can be replaced by the abstract operator again.

Thus we arrive at

$$\Psi^{(\pm)} = \Omega_\pm \phi = \phi - \lim_{\epsilon \downarrow 0} \int_0^\infty (H - E \pm i\epsilon)^{-1} V dP(E) \phi. \tag{32}$$

which bears great similarity with the LS equation.

3.2.1 Final step to the LS equation

At first glance Eq. (20) looks better than the LS equation, as it is a direct expression for some scattering wave packet $\Psi^{(\pm)}$ rather than an integral equation for it. However, it contains $(H - E \pm i\epsilon)^{-1}$, which usually is rather inaccessible to computation.

By simple algebraic manipulations one can derive the LS from (20). We use a slightly more abstract from of getting there, as it emphasizes the symmetric roles of H_0 and H in scattering theory. We interchange $H_0 \leftrightarrow H$

$$H, H_0, H - H_0 =: V \to H' = H_0, H_0' = H, H' - H_0' = H_0 - H = -V \tag{33}$$

to write

$$\phi^{(\pm)} = \psi + \lim_{\epsilon \downarrow 0} \int_0^\infty (H_0 - E \pm i\epsilon)^{-1} V dP_H(E) \psi, \quad \psi \in P_{ac}(H)\mathcal{H}. \tag{34}$$

Next remember that the signs $\pm$ just indicate whether the $\phi^{(\pm)}$ and ψ are mapped by going through the the remote past or future. That is, we can just as well move $\pm$ from ϕ back to ψ, leading to

$$\psi^{(\pm)} = \phi - \lim_{\epsilon \downarrow 0} \int_0^\infty (H_0 - E \pm i\epsilon)^{-1} V dP_H(E) \psi^{(\pm)}. \tag{35}$$

3.2.2 The LS equation in position space

In position space, the LS equation takes the form

$$\psi^{(\pm)}(\vec{r}) = e^{i\vec{k}\vec{r}} - \int_{\mathbb{R}^3} dr^{(3)} \frac{e^{\mp ik|\vec{r}-\vec{r}'|}}{4\pi|r-r'|} V(\vec{r}) \psi^{(\pm)}(\vec{r}'). \tag{36}$$

where we recognize the form of the solution $\psi^{(\pm)}(\vec{r})$ as a plane wave plus a superposition of spherical waves.

Problem 3.2: Green's function in position space Compute the function

$$G_\pm(\vec{r}, \vec{r}') = \frac{1}{(2\pi)^3} \int d^{(3)}k \frac{e^{i\vec{k}(\vec{r}-\vec{r}')}}{k_0^2 - k^2 \pm i\epsilon} = -\frac{1}{4\pi} \frac{e^{\pm ik_0|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|}$$

(We use the physicists' convention not to explicitly write the $\lim_\epsilon$).
Hint: Use polar coordinates, expansion of a plane wave into spherical Bessel functions, integrate over the angle, use the residue theorem for what remains.

4 S-matrix

As a first step for connecting to experimental observables, we ask: what is the probability of finding a system, that in the remote past was a free wave packet state χ_i, say with a narrow momentum wave-packet around a given $\vec{k}$, in the free momentum wave packet χ_e around $\vec{q}$ after scattering. For that we map the two wave free wave packets into the actual scattering solutions ϕ_i and ϕ_e by applying the scattering operators Ω_- and Ω_+, respectively. Note that we choose two different signs, as we want to map the incoming free wavepacket χ_i to the scattering wave packet $\phi_i = \Omega_-\chi_i$, such that they are equal at the remote past, and conversely $\phi_e = \Omega_+\chi_e$ with mapping in the remote future.

By general quantum theory, our probability is

$$\langle\varphi_i|\varphi_e\rangle\langle\varphi_e|\varphi_i\rangle. \tag{37}$$

All we need to know is

$$\langle\varphi_e|\varphi_i\rangle = \langle\Omega_+\chi_e|\Omega_-\chi_i\rangle = \langle\chi_e|\Omega_+^*\Omega_-\chi_i\rangle =: \langle\chi_e|S\chi_i\rangle \tag{38}$$

The operator $S := \Omega_+^*\Omega_-$ is traditionally called S**-matrix** and obviously contains all information that we are interested in for a scattering experiment. For asymptotic complete problems, it is a unitary map between the *ac* spectral parts of the free time evolution $S : P_{ac}(H_0) \to P_{ac}(H_0)$.

Note that in this reasoning the relation to the cross section is still a bit murky, as we do not clearly specify at which point of their evolution we compare the two scattering wave packets. In the limit of infinitely narrow wave packets, this question disappears: in this limit, the particles become completely delocalized and it does not matter, at which time we compare the wave packets, the particles are "always everywhere". We will not explicitly go through the rather tedious exercise of actually taking the limit.

4.1 Mapping free to free eigenspaces

The S-matrix is

$$\Omega_+^\dagger\Omega_- = (\Omega_+)^{-1}\Omega_- := S. \tag{39}$$

The inverse is to be understood between the $\mathcal{H}_{ac}$ subspaces. This should be something like the limit

$$\lim_{t\to\infty}[U(-t)U_0(t)]^{-1}[U(t)U_0(-t)] = \lim_{t\to\infty} U_0(-t)U(2t)U_0(-t)] \tag{40}$$

i.e. bring a free packet sufficiently far into the past, let it interact for sufficiently long time (into the future), propagate the free packet it back into the present: generate the effect of scattering as a mapping between free wave packets.

Some desirable properties of the S-matrix:

- is unitary (asymptotic completeness)
- it "inherits" symmetries from H and H_0.
- it conserves energy - intertwining relation

4.1.1 Physics notation

$\Omega_\pm$ in the spectral representation of H_0

$$\Omega_\pm = 1 - \lim_{\epsilon \downarrow 0} \int_0^\infty (H - E \pm \imath\epsilon)^{-1} V \delta(H_0 - E) dE \tag{41}$$

with E in $\sigma_{ac}(H_0)$. Meaning of $\delta(H_0 - E)$ (through spectral representation of H_0, Dirac notation)

$$\delta(H_0 - E) = \sum\!\!\!\!\!\!\int_\alpha |E, \alpha\rangle\langle E, \alpha| \tag{42}$$

with α independent of E numbering the degenerate (generalized) eigenfunctions for energy E.

Note: this operator takes functions out of the Hilbert space, within the framework discussed in the lectures, it is not terribly well-defined. Formally, we can turn it into a well-defined operator by integrating over a Borel-set $B \subset \mathbb{R}$

$$Q_B = \sum\!\!\!\!\!\!\int_\alpha \int_B dE |E, \alpha\rangle\langle E, \alpha|. \tag{43}$$

This is a map from the Borel sets into the linear operators, actually Q_B is the projector valued measure for B associated with the spectral representation of H_0.

A priori, the index α can be discrete or continuous. It could be, e.g., the space of directions $\vec{k}/|\vec{k}|$, i.e. the angles. In this case we have a discrete basis $\alpha = (l, m)$ Then we see that actually

$$Q_B = \sum_{l,m} Q_{B,l,m} \tag{44}$$

4.2 Spectral representation of S

As for the $\Omega_\pm$, we have the S-matrix in the spectral representation of H_0:

$$S = \lim_{\epsilon \downarrow 0} \int_0^\infty dE \left\{1 - 2\pi\imath\delta(H_0 - E)\left[V - V(H - E + \imath\epsilon)^{-1}V\right]\right\}\delta(H_0 - E). \tag{45}$$

Energy conservation $H_0 S = S H_0$ implies that S is a function of H_0, i.e. in the spectral representation is a multiplication with respect to E. It may still connect different α, though (after all, we are free to choose the basis in the space of fixed E spanned by the $|E, \alpha\rangle$.

4.2.1 Scattering phases $\delta_l(k)$

In the rotationally symmetric case, $S = \bigoplus_{lm} S_l$ we know that l, m is not changed and therefore can be parameterized by the "scattering phases", conventionally written with $k = \sqrt{E}$:

$$S|E, l, m\rangle = e^{2i\delta_l(k)}|E, l, m\rangle \tag{46}$$

(Remember that S_l for rotationally symmetric problems is independent of m)

Derivation

$$\begin{aligned} S &= s\text{-}\lim_{\epsilon\downarrow 0}\epsilon\int_0^\infty dt\int_0^\infty\int_0^\infty dEdE'\delta(H_0-E)e^{-it(H-\frac{E+E'}{2}-i\epsilon)}\delta(H_0-E') \\ &= s\text{-}\lim_{\epsilon\downarrow 0}\epsilon\int_0^\infty\int_0^\infty dEdE'\delta(H_0-E)\frac{-i\epsilon}{H-\frac{E+E'}{2}-i\epsilon}\delta(H_0-E') \end{aligned}$$

Problem 4.3: Resolvent equation An important identity for $H = H_0 + V$:

$$(H-z)^{-1} = (H_0-z)^{-1} - (H_0-z)^{-1}[V - V(H-z)^{-1}V](H_0-z)^{-1} \tag{47}$$

Verify this!

The first term evaluates to

$$s\text{-}\lim_{\epsilon\downarrow 0}\epsilon\int_0^\infty dt\int_0^\infty\int_0^\infty dEdE'\delta(H_0-E)\frac{-i\epsilon}{H_0-E-i\epsilon}\delta(H_0-E') = \int dE\delta(H_0-E) \tag{48}$$

Further

Problem 4.4: δ-function

$$\lim_{\epsilon\downarrow 0}\frac{-i\epsilon}{[(E-E')/2-i\epsilon][(E'-E)/2-i\epsilon]} = 2\pi i\delta(E-E'). \tag{49}$$

By this, one can integrate over E' for the second term and one arrives at Eq. (45).

4.2.2 The T-matrix

Let ψ, ψ be two wave packets. The matrix elements of the S-matrix can be written as

$$\langle\psi, S\psi\rangle = \langle\psi,\psi\rangle - 2i\pi\int d^{(3)}k\,\psi(\vec{k})^* t(\vec{k},\vec{k}')\delta(\vec{k}^2-\vec{k}'^2)\psi(\vec{k}') \tag{50}$$

where $\psi(\vec{k})$ is the representation of ψ in $\vec{k}$-space with the matrix elements of the **T-matrix**

$$T(z) := V - V(H-z)^{-1}V \tag{51}$$

taken "on shell", i.e. $z = E + i\epsilon$:

$$t(\vec{k},\vec{k}') = \langle\vec{k}|V - V(H-E-\imath\epsilon)^{-1}V|\vec{k}'\rangle, \tag{52}$$

where $|\vec{k}\rangle = \exp(i\vec{k}\vec{x})/(2\pi)^{3/2}$ are the δ-normalized plane waves $\langle\vec{k}|\vec{k}'\rangle = \delta^{(3)}(\vec{k}-\vec{k}')$ and $\psi(k) = \langle\vec{k}|\psi\rangle$. Note

$$V - V(H-E-\imath\epsilon)^{-1}V = V\Omega_-(E) = \Omega(E)_+^\dagger V \tag{53}$$

It essentially is the same as the **scattering amplitude** $f(k, \vec{n}, \vec{n}')$

$$f(k, \vec{n}, \vec{n}') = -(2\pi)^2 t(k\vec{n}, k\vec{n}') \tag{54}$$

whose square gives the differential cross section:

$$\sigma(\vec{k}, \vec{k}') = |f(k, \vec{n}, \vec{n}')|^2. \tag{55}$$

4.2.3 Analyticity of $t(\vec{k}, \vec{k}')$

$t(\vec{k}, \vec{k}')$ contains the relevant scattering information. Also, it is a smooth function of $\vec{k}, \vec{k}'$ where solutions of the LS equation exist. The $t(\vec{k}, \vec{k}')$ are analytic functions of $k = |\vec{k}| = |\vec{k}'|$ on the complete upper half complex plane up to the real k-axis. For potentials that decay exponentially (Yukawa type) one can analytically continue into the lower half plain.

4.3 Scattering cross section

Typical scattering experiments can be described as aiming a macroscopically broad beam onto a microscopic target or a statistical ensemble of microscopic targets. What is measured is at which angle one finds scattering products. In the scattering processes that we have discussed so far, there is only a single particle and usually there is a time-independent Hamiltonian. In that case energy is conserved and the only parameter that needs to be measured is the angle at which one finds a particle. The number of particles found at a certain scattering angle, if one particle impacts per surface unit is the "scattering cross section". It tells us, how many particles out of a broad beam are deflected into a given direction.

The scattering cross section is the main way how to relate experimental data to experiment. This is why we will go through its slightly cumbersome derivation from fundamental scattering theory. (The derivation can also be found in Thirring, chap 3.6).

On the microscopic level, we have all scattering information in the S matrix. To compute the scattering cross section, we need to model the beam of particles with a macroscopic diameter. We assume that the particles in the beam are independent of each other. This means in particular that their quantum phases are in no fixed relation to each other. The beam is considered to be transversally incoherent. In that case, scattering a beam from a microscopic target is equivalent to repeating a single scattering process and averaging over all impact parameters, i.e. the distance at which a single wave packet passes the target. We *do* assume that all particles of the beam have the same energy, that is, the beam is "mono-energetic": the beam is time-coherent.

We will work in the spectral representation of H_0. A single momentum wave packet with an approximate momentum $\vec{k}_0 = (0, 0, k_0)$ is described by $\phi(\vec{k})$ where $\int d^{(3)}k |\phi(\vec{k})|^2 = 1$ and $\phi(\vec{k})$ is non-zero only in the vicinity of $\vec{k}_0$. We can shift this wave packet in $\vec{x}$-space by a vector $\vec{a} = (a_x, a_y, 0)$ perpendicular to $\vec{k}_0$ by the multiplication $\phi(\vec{k}) \to \phi(\vec{k}) e^{\imath \vec{a}\vec{k}}$. Remember that multiplication by $e^{\imath \vec{a}\vec{k}}$ in $\vec{p}$-space is equivalent to applying the shift-operator $\exp(\imath \vec{a}\vec{p})$ in $\vec{x}$-space. The scattered shifted wave packet is

$$\psi_{\vec{a}} = S\phi_{\vec{a}}. \tag{56}$$

The probability of finding in the scattered wave packet momenta $\vec{k}$ in a certain solid angle $\Delta\Omega$ and within a range of magnitudes Δk is

$$\int_{\Delta\Omega} d\Omega \int_{\Delta k} dk k^2 |\psi_{\vec{a}}(\vec{k})|^2 \tag{57}$$

Here we use polar coordinates k, θ, ϕ :

$$\vec{k} = k \begin{pmatrix} \sin\theta\cos\phi \\ \sin\theta\sin\phi \\ \cos\theta \end{pmatrix} \tag{58}$$

and the notation for the "solid angle" $\Delta\Omega$ around some $\Omega_1 = (\theta_1, \phi_1)$

$$\int_{\Delta\Omega} d\Omega \int_{\Delta k} dk = \int_{\theta_1-\Delta\theta}^{\theta_1+\Delta\theta} d\theta \sin\theta \int_{\phi_1-\Delta\phi}^{\phi_1+\Delta\phi} d\phi \int_{k_1-\Delta k}^{k_1+\Delta k} dk \tag{59}$$

To model the beam, we average the probability by integrating $\vec{a}$ over some large beam cross section A and dividing by the surface area

$$\frac{1}{A} \int_A d^{(2)}a \int_{\Delta\Omega} d\Omega \int_{\Delta k} dk k^2 |\psi_{\vec{a}}(\vec{k})|^2 \tag{60}$$

If $\vec{k}_0$ is non-zero, the particle is certain to pass somewhere through the surface perpendicular to $\vec{k}_0$. The probability for a particle to pass one surface unit is therefore $1/A$. We divide by $1/A$, as we want to find scattering for a beam with one particle per unit surface. Finally, we assume that the angle $\Delta\Omega$ is far enough from the beam direction $(0, 0, 1)$ such that no *unscattered* particles from the beam directly fall into it, i.e. $\int_{\Delta\Omega} |\phi(\vec{k})|^2 = 0$. With this, 1 in the spectral representation of the S-matrix (45) does not give a contribution. The cross section is

$$\begin{aligned} \sigma(\vec{k}, \vec{k}') &:= \int_A d^{(2)}a \int_{\Delta\Omega} d\Omega \int_{\Delta k} dk k^2 |\psi_{\vec{a}}(\vec{k})|^2 \\ &= \int_A d^{(2)}a \int_{\Delta\Omega} d\Omega \int_{\Delta k} dk k^2 \left| \int d^{(3)}k' \int dE' \delta(\frac{k^2}{2} - E') t(\vec{k}, \vec{k}') \delta(\frac{k'^2}{2} - E') \phi(\vec{k}') e^{\imath\vec{a}\vec{k}'} \right|^2 \end{aligned}$$

where we have defined

$$t(\vec{k}, \vec{k}') = 2\pi \langle \vec{k} | V - V(H - k^2/2 - \imath\epsilon)^{-1} V | \vec{k}' \rangle. \tag{61}$$

This becomes

$$\begin{aligned} &= \int_A d^{(2)}a \int_{\Delta\Omega} d\Omega \int_{\Delta k} dk k^2 \int d^{(3)}k' \int dE' \int d^{(3)}k'' \int dE'' && (62) \\ &\quad \delta(\frac{k^2}{2} - E') \delta(\frac{k'^2}{2} - E') \delta(\frac{k^2}{2} - E'') \delta(\frac{k''^2}{2} - E'') && (63) \\ &\quad t^*(\vec{k}, \vec{k}') t(\vec{k}, \vec{k}'') \phi^*_{\vec{a}}(\vec{k}') \phi_{\vec{a}}(\vec{k}'') e^{\imath\vec{a}(\vec{k}'' - \vec{k}')} && (64) \end{aligned}$$

Integration over E' and E'' leads to

$$\begin{aligned} &= \int_A d^{(2)}a \int_{\Delta\Omega} d\Omega \int_{\Delta k} dk k^2 \int d^{(3)}k' \int d^{(3)}k'' && (65) \\ &\quad \delta(\frac{k^2}{2} - \frac{k'^2}{2}) \delta(\frac{k^2}{2} - \frac{k''^2}{2}) t^*(\vec{k}, \vec{k}') t(\vec{k}, \vec{k}'') \phi^*_{\vec{a}}(\vec{k}') \phi_{\vec{a}}(\vec{k}'') e^{\imath\vec{a}(\vec{k}'' - \vec{k}')} && (66) \end{aligned}$$

Integration over $dkk^2 = d(\frac{k^2}{2})k$ gives

$$= \int_A d^{(2)}a \int_{\Delta\Omega} d\Omega k \int d^{(3)}k' \int d^{(3)}k'' \tag{67}$$

$$\delta(\frac{k'^2}{2} - \frac{k''^2}{2}) t^*(\vec{k},\vec{k}') t(\vec{k},\vec{k}'') \phi^*_{\vec{a}}(\vec{k}') \phi_{\vec{a}}(\vec{k}'') e^{\imath\vec{a}(\vec{k}''-\vec{k}')} \tag{68}$$

For the integral over $d^{(2)}a$ we observe that

$$\int_A d^{(2)}a e^{\imath\vec{a}(\vec{k}''-\vec{k}')} = (2\pi)^2 \delta(k'_x - k''_x)\delta(k'_y - k''_y) \tag{69}$$

and obtain

$$= (2\pi)^2 \int_{\Delta\Omega} d\Omega k \int d^{(3)}k' \int d^{(3)}k'' \tag{70}$$

$$\delta(\frac{k'^2}{2} - \frac{k'^2}{2}) \delta(k'_x - k''_x)\delta(k'_y - k''_y) t^*(\vec{k},\vec{k}') t(\vec{k},\vec{k}'') \phi^*_{\vec{a}}(\vec{k}') \phi_{\vec{a}}(\vec{k}'') \tag{71}$$

The three 1-dimensional deltas combine to

$$\delta(\frac{k'^2}{2} - \frac{k'^2}{2}) \delta(k'_x - k''_x)\delta(k'_y - k''_y) = \delta^{(3)}(\vec{k}' - \vec{k}'')/k'_z \tag{72}$$

and another integral goes away

$$= (2\pi)^2 \int_{\Delta\Omega} d\Omega \int d^{(3)}k' |t(\vec{k},\vec{k}')|^2 |\phi_{\vec{a}}(\vec{k}')|^2 \frac{k'}{k'_z} \tag{73}$$

Now we use that $\phi(\vec{k})$ is very narrowly concentrated around $\vec{k}_0$ such that $k_0 \approx k' \approx k'_z$ and $t(\vec{k},\vec{k}') \approx t(\vec{k},\vec{k}_0)$ for small range where the integral is non-zero. Also we use $||\phi|| = 1$

$$= (2\pi)^2 \int_{\Delta\Omega} d\Omega |t(\vec{k},\vec{k}_0)|^2 \tag{74}$$

To connect to conventional notation, we introduce the
Scattering amplitude

$$f(\vec{k},\vec{k}_0) := -(2\pi)t(\vec{k},\vec{k}_0) = -(2\pi)^2 \langle\vec{k}|V - V(H - k^2/2 - \imath\epsilon)^{-1}V|\vec{k}_0\rangle \tag{75}$$

and write the **scattering cross section**

$$\frac{d\sigma(\vec{k},\vec{k}_0)}{d\Omega} = |f(\vec{k},\vec{k}_0)|^2 \tag{76}$$

If our H_0 is the free time-evolution with the δ-normalized scattering functions $|\vec{k}\rangle = e^{\imath\vec{k}\vec{x}}/(2\pi)^{3/2}$, the scattering amplitude is expressed in terms of the plane wave matrix elements

$$f(\vec{k},\vec{k}_0) = -(2\pi)^{-1} \langle e^{\imath\vec{k}\vec{x}}|V - V(H - k^2/2 - \imath\epsilon)^{-1}V|e^{\imath\vec{k}_0\vec{x}}\rangle \tag{77}$$

Post- and prior forms: Using the Møller operator equation in the form

$$\Psi^{(\pm)}(\vec{k}) = \Omega_\pm|\vec{k}\rangle = \left[1 - (H - \vec{k}^2/2 \pm \imath\epsilon)^{-1}V\right]|\vec{k}\rangle \tag{78}$$

the scattering amplitude can also be written as

$$f(\vec{k},\vec{k}_0) = -(2\pi)^2 \langle\vec{k}|V|\Psi^{(-)}(\vec{k}_0)\rangle \quad \text{“post” form} \tag{79}$$

$$= -(2\pi)^2 \langle\Psi^{(+)}(\vec{k})|V|\vec{k}_0\rangle \quad \text{“prior” form} \tag{80}$$

Here the standard bra-ket notation can be deceptive: the Møller operators are not self-adjoint, so it is intended that they are applied to the right, i.e.

$$\begin{aligned}\langle\Psi^{(+)}(\vec{k})|V|\vec{k}_0\rangle &= \langle\Omega_+\vec{k}|V|\vec{k}_0\rangle = \langle\vec{k}|\Omega_+^\dagger V|\vec{k}_0\rangle \\ &= \langle\vec{k}|[1-(H-k^2/2+i\epsilon)V]^\dagger V|\vec{k}_0\rangle \\ &= \langle\vec{k}|[1-V(H-k^2/2-i\epsilon)]V|\vec{k}_0\rangle\end{aligned}$$

The two forms above are mathematically equivalent and, in case of potential scattering, also completely equivalent in practical use. Differences appear when one approximates the scattering states $\Psi^{(\pm)}$. In the case of multi channel scattering one scattering solution, e.g. $\Psi^{(+)}$, may be easier to approximate that the other. Consequently, in approximate form, post or prior may be a better choice for approximating $f(\vec{k},\vec{k}')$.

The **total cross section** is the integral of the differential cross section over all scattering angles. As $|\vec{k}| = |\vec{k}_0|$ we can write in polar coordinates $f(\vec{k},\vec{k}_0) = f(k,\Omega,\Omega_0)$ and integrate over the scattering angle Ω

$$\sigma_{tot} = \int d\Omega |f(k,\Omega,\Omega_0)|^2 \tag{81}$$