Notes related to “Scattering theory”

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USE WITH CAUTION — DISCLAIMER

These notes are compilation of my “scribbles” (only SCRIBBLES, although typeset in LaTeX). There absolutely no time to unify notation, correct errors, proof-read, and the like. Your primary source must by your own notes.

For now, it is only an outline to list a few of the topics that will be covered. The notes will be partially be filled in as the lecture proceeds.

Contents summary

The lecture gives an introduction to quantum scattering theory, covering contents of practical importance such as the Lippmann-Schwinger equation and Born series, scattering amplitude and cross section, multi-channel scattering and re-arrangement, resonances and inverse scattering. The somewhat distinct properties of Coulomb scattering will be presented. Occasionally, computational examples will be used for illustrating paper-and-pencil theory. Fundamental concepts that underly scattering theory, such as the Moeller operators and “asymptotic completeness”, the S-matrix, and spectral properties of the Hamiltonians, will be laid out with some mathematical rigor, but mostly without rigorous proofs. For the more practical content, the main reference is Taylor’s book “Scattering Theory”, while formulation and mathematical background will be in the spirit of Thirring’s Course in mathematical physics: Quantum mechanics of atoms and molecules, with occasional references to Reed and Simon.

Purpose of the lecture

Scattering theory is notoriously difficult teach, let alone to implement in serious practical application. Contrary to quantum mechanics of bound states, simple analogies to discrete vector spaces can be misleading.

Literature

The course of the lecture is strongly inspired by
W. Thirring - Lehrbuch der Mathematischen Physik

The part on unbounded operators follows closely
G. Teschl - Mathematical Methods in Quantum Mechanics

For basic reference we will largely use
Reed/Simon - Methods of Modern Mathematical Physics

Further literature will we given for selected topics.
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1 Scattering phenomena and basic concepts

We do not, in general, approach microscopic systems with microscopic instruments. Neither do we, in general, observe processes directly on the time scale on which they evolve. There are notable exceptions to this — such as the scanning tunneling microscopy in space, or attosecond science in time — but the bulk of our knowledge about the microscopic world is drawn from analysis of measurements at lab distances and times much larger than the inherent time-scale of a process. Scattering theory is about this connection of macroscopic measurement to microscopic events. Considering large times and distances as “practical” infinity, the simplification from taking the limit to mathematical infinity exposes the simplest possible representation of actual measurement.

“Simplest possible”, unfortunately, is a relative statement here, and the unwieldiness of scattering theory results in its neglect in standard curricula, notwithstanding its extraordinary conceptual and practical importance.

The abstract procedure of a scattering experiment is simple: direct a macroscopic beam (of light or other particles, the “projectiles”) onto a “target” (usually an ensemble of microscopic particles, sometimes even single particles), and detect any changes in the beam or fragments of the target that are emitted.

1.1 Rutherford cross-section formula

In that historical experiment of 1909, the beam were the alpha-particles from the decay of Radium (discovered just a few years earlier), the target a gold foil. The result was quite unexpected and could be explained as scattering by point-like Coulomb charges, upsetting the contemporary concepts of atomic structure.

The celebrated scattering formula can be derived by simple means, if not with much mathematical rigor. Ironically, it is not amenable to standard methods of scattering theory as the Coulomb potential “never ends”, a fact that has disquieted cosmologists on earlier occasions. (For it to really “end” it would need to decay as $r^{-1-\epsilon}$ at the least).

The problem is similar in quantum and classical mechanics, and for a first exercise you should remind yourself of the following formula’s deriva-
The differential cross-section for scattering two charge, point-like particles is
\[ \frac{d\sigma}{d\Omega}(E, \theta) = \left( \frac{Z_1 Z_2 e^2}{4E \sin^2 \frac{\theta}{2}} \right)^2. \] (1)

**Problem 1.1: Center-of-mass to lab frame** Derive the transformation formula for the cross section.

\[ \frac{d\sigma}{d\Omega_{\text{lab}}} = \frac{d\sigma}{d\Omega_{\text{cm}}} \left( 1 + 2\lambda \cos \theta_{\text{cm}} + \lambda^2 \right)^{3/2} \left| 1 + \lambda \cos \theta_{\text{cm}} \right| \] (2)

with \( \lambda = m_p/m_t \) the ratio of projectile to target mass and \( \theta_{\text{cm}} \) the angle in the center-of-mass system. Specify the arguments in the cross-section function.

**Hint:** All that is needed is to transform the partial derivatives
\[ \frac{\partial}{\partial\Omega_i} = \frac{\partial\Omega_i}{\partial\Omega} \frac{\partial}{\partial\Omega} \]

**Problem 1.2: First Born approximation** A popular method to investigate scattering is the so-called “first Born approximation”. Its main part is to compute the “scattering amplitude” in the first Born approximation \( f^{(1)} \) as
\[ f^{(1)}(\vec{k}, \vec{k}_i) = -(2\pi)^2 \langle \vec{k} | V | \vec{k}_i \rangle, \] (3)
where \( |\vec{k}\rangle \) and \( |\vec{k}'\rangle \) are \( \delta \)-normalized plane waves. Compute that integral for the Yukawa potential
\[ V(r) = V_0 \frac{e^{-\mu r}}{r}, \quad \mu > 0. \] (4)

The modulus squared of the scattering amplitude is the cross section
\[ \frac{d\sigma(\vec{k}, \vec{k}_i)}{d\Omega} = \left| f(\vec{k}, \vec{k}_i) \right|^2. \] (5)

(a) How does the first Born cross section depend on the sign of \( V_0 \)?
(b) How does the cross section behave with \( |\vec{k}| \to 0 \)?
(c) What is the total cross section
\[ \int_{-1}^{1} d\cos \theta \int d\phi |f^{(1)}(\vec{k}, \vec{k}_0)|^2? \] (6)
\[ \theta \text{ and } \phi \text{ are the polar angles of } \vec{k} = |\vec{k}_0|(\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta). \]

(d) What is the cross-section in the limit \( \mu \to 0? \)

**Hint:** In polar coordinates, the integral can be readily computed.

### 1.2 Cross-section

This introduces the important concept of cross section, which has an immediate interpretation for measurement: suppose we have beam of particles incident from a fixed direction (say the z-axis) onto a target (one of the gold nuclei in the foil) and the energies are uniformly distributed in as (differentially) small bin \([E, E + \Delta E]\). Our beam being macroscopic, we cannot make any statement about where the target nucleus is located across the beam, other than we would like to ensure that alpha particles pass at all reasonable microscopic distances of it. We assume that the beam is homogeneous across all possible target locations, i.e. the density of flux is equal everywhere. We characterize the incident beam by (a) the energy \(E\) and (b) the number of particles passing through a unit surface perpendicular to the beam direction per unit time: \(\rho_i(E)\). The measurement consists in detecting particles in all directions relative to the z-direction. As our microscopic system, the gold atom, can be idealized as a point particle and is spherically symmetric (as we know today), the only relevant angle is the polar angle \(\theta\) of the spherical coordinate system. Counting the number of “scattered” particles \(N_s\) per unit time found at some solid angle \(\Omega = \theta, \phi : [\theta, \theta + \Delta \theta] \times [\phi, \phi + \Delta \phi] =: [\Omega, \Omega + \Delta \Omega], \) (7)
we will find
\[ N_s = \rho_i \frac{d\sigma}{d\Omega}(E, \theta) \Delta \Omega. \] (8)

We see that the name “cross-section” is fitting, as \(d\sigma/d\Omega\) has the dimension of a surface. You can consider it as the “size” of the surface taken out from the beam by that target and re-directed into \(\Omega\).
The pathologies of Coulomb scattering show already here: we might want to ask how many particles are “taken out of the beam” and but then released in beam direction, i.e. $\theta = 0$, the formula gives an answer: infinitely many, it diverges. At first glance a nonsensical result, but it is actually true: our idealization of the beam as homogenous implies that it is “infinitely wide”, so after we have taken all finite pieces for scattering into any finite angle, there still remains infinitely much beam, which however does not pass without noticing the presence of the Coulomb potential: there will be some delay (or advance) of the particle, as it passes the repulsive (or attractive) Coulomb center, not matter at which distances: the forward scattering amplitude of the Coulomb potential is infinite: it transversally is “infinitely large”.

“Reasonable”, i.e. short range potentials, do not have infinite cross sections: this actually is true for any potential falling off stronger than $1/r^2$ at large distances check.

1.3 Partially differential, fully differential, and total cross section

The above example allows to first introduce the important concepts fully differential, partial, and total cross section. To the extent that we are dealing (in our idealization) with spinless point particles, the Rutherford cross section differentiates all observables at large times: direction and energy. The cross section is “fully differential”.

Suppose we cannot measure energy $E$, but only the angle $\Omega$. Counting the particles at that angle results in a partially differential cross-section w.r.t. to angles (the dependence on $\phi$ is constant, trivially):

$$\frac{d\sigma}{d\Omega}(\Omega) = \int_0^{\infty} dE \frac{d\sigma(E, \theta)}{d\Omega}$$

Likewise, one could integrate over angles and differentiate over energies:

$$\sigma(E) = \int d\Omega \frac{d\sigma(E, \theta)}{d\Omega} = \int_0^{2\pi} \int_0^{\pi} d\theta \sin \theta \frac{d\sigma(E, \theta)}{d\Omega},$$

which is infinite for the Coulomb scattering, i.e. it is not a good number to ask for: Coulomb always scatters.

Finally, if we ask whether there is any scattering at all, i.e. we integrate over all energies and angles, we get the total cross section $\sigma_t$. We have
noticed already that the total cross section for the Coulomb potential is infinite.

1.4 Center-of-mass vs. lab frame cross-section

The Rutherford cross-section formula holds for a fixed, infinite mass target, or, alternatively, for a in rest frame of the center of mass. In the case of gold atom and alpha-particles, the mass ratio is about 1/60, and although the approximation is not bad, an accurate description require transformation into the center of mass frame moving into the lab-frame by the formula

\[ \frac{d\sigma}{d\Omega_{\text{lab}}} = \frac{d\sigma}{d\Omega_{\text{cm}}} \left( \frac{1 + 2\lambda \cos \theta_{\text{cm}} + \lambda^2}{1 + \lambda \cos \theta_{\text{cm}}} \right)^{3/2} \] (11)

This is left as an entertaining exercise to get you started on the use of calculus in this lecture.

1.5 Observables in scattering experiments

Detectors can register:

- direction of emission,
- kinetic energy of arriving particle,
- possibly its internal state (spin, excitation state, mass),
- arrival times.

Note that resolution of arrival times is on a macroscopic time scale (even nano-seconds are “macroscopic” in relation to most microscopic time scales). These times, is measured, are usually used to determine kinetic energy from knowing time of emission and distance to the point of arrival (“time of flight” detector).

1.6 Potential scattering, multi-channel scattering, break-up, and rearrangement

The kinematic situation of Rutherford scattering is the simplest possible: a particle gets deflected from a rotationally symmetric scatterer which appears (in center of mass) as a potential. There is no source or sink of energy,
energy is conserved. This is a case of potential scattering. Rotational symmetry reduces the problem to an (infinite) set of one-dimensional problems, each for a given angular momentum, the partial waves.

This a standard situation, also for example in scattering of atoms and molecules. Rotationally symmetric potential scattering is the case of two atoms, say $He$ and $Ar$ at energies that are so low that the systems cannot be transferred into excited states:

$$He + Ar \rightarrow He + Ar.$$  

(12)

The lowest excitation energy of $Ar$ is about 12 eV, below that energy the above process can be considered as potential scattering (a cleaner case would be electron-proton scattering).

Potential scattering also includes scattering without rotational symmetry, which already poses a significant complication, e.g. scattering from molecules, say $H_2$:

$$He + H_2 \rightarrow He + H_2.$$  

(13)

Here potential scattering is an adequate picture only at the lowest energies, as $H_2$ can be brought easily into rotation, with the lowest rotational excitation at $\gtrsim 10 meV$.

If the target can assume different states (say the ground or excited states of an atom or a nucleus, labelled as $A^{(n)}$), a new layer of complexity is added. We have processes where scattering changes the state of the target:

$$He + A^{(m)} \rightarrow He + A^{(n)}.$$  

(14)

We enter the scattering process in one “channel” $(m)$, but leave through a different channel $(n)$. We need to differentiate the multi-channel scattering cross-section

$$\frac{d\sigma(E_{in}, m, n, \Omega)}{d\Omega},$$  

(15)

depending on the ingoing kinetic energy $E_{in}$, the initial and final state labels $m, n$, and the scattering angle. The outgoing kinetic energy is, of course,

$$E_{out} = E_{in} + E_m - E_n,$$  

(16)
where $E_m, E_n$ are the internal energies of $A^{(m)}, A^{(n)}$, respectively. For example, $E_{in} > 12eV$, we can excite $Ar(3s^23p^6) \rightarrow Ar(3s^23p^54s)$, and the center-of-mass $E_{out} = E_{in} = 11.6eV$.

Multi-channel scattering is very common in experimental practice, but it entails already a significant mathematical complication. Things get worse, when projectile and/or target can disintegrate, as any of the following examples of break up reactions

$$He + H_2 \rightarrow He + H + H$$  \hspace{1cm} (17)

$$He + H_2 \rightarrow He + H + p + e$$  \hspace{1cm} (18)

$\vdots$ \hspace{1cm} (19)

$He$ with its binding energy of about 24 eV will remain intact at energies below that, but may and will disintegrate at higher scattering energies.

A further variation of the situation is that of both projectile and target rearrange into new compounds. An important such process is electron capture in nuclear physics, where, for example an instable $C^{11}$ nucleus captures and electron and, under emission of a neutrino, converts to $Bo^{11}$. The re-arrangement of constituents, in the end, is essence of reactive chemistry and as such of utmost importance to life. But the underlying processes do not usually occur in typical scattering setups.

A fully differential cross section in such more complex situations can be defined as follows: Given an ensemble of incident sub-system/particles characterized by \{\vec{k}_i, s_i, i = 1, \ldots, I\} with momenta \vec{k}_i, internal states $s_i$ (e.g. spin, constituents, excitation state etc., if any), and flux $F_i$ (number of such subsystems per time per surface), one measures the number $N_e$ of sub-systems/particles emitted per time into momenta and internal states \{\vec{q}_e, s_e, e = 1, \ldots, E\}. The fully differential cross section is the ratio

$$\sigma(\vec{k}_1, s_1, \ldots \vec{k}_I, s_I; \vec{q}_1, s_1, \ldots \vec{q}_E, s_E) = \frac{N_e}{F_i}$$  \hspace{1cm} (20)

This is what we ultimately need to know for comparison with observation. We also see that this is an enormous amount of information, both, to measure and to compute. Handling such complex situations is commonplace in particle physics. In atomic and molecular physics there also exists a powerful instrument that delivers such complex data: the COLTRIMS (Cold
Target Recoil Ion Momentum Spectroscope), where all outgoing momenta can be collected.

For potential scattering we possess mature and well-founded mathematical theory that also allows practical implementation. As complexity increases, mathematical rigor quickly disintegrates and practical implementation becomes cumbersome and rapidly deteriorates in accuracy. The lecture will concentrate on the rigorous part, only formulating, rarely solving the problems of the more complex situations.

1.7 Resonances and decay

Scattering cross sections can and do very often show striking, well-isolated peaks. The phenomenon is rather generic and occurs in the eerie world of elementary particle physics as well as quantum-toddler’s square-well potential. The peak occurs around a certain resonance energy $E_r$ (and possible other parameters as angular momentum or spin), and it has a certain width $\Gamma$. Two prominent line-shapes are the Lorentzian (or Breit-Wigner) profile

$$\sigma(E, E_r, \Gamma) = \sigma_0 \frac{(\Gamma/2)^2}{(E - E_r)^2 + (\Gamma/2)^2}$$

and the slightly more complex Fano profile

$$\sigma(E - E_r) = \sigma_0 \frac{(q\Gamma/2 + E - E_r)^2}{(E - E_r)^2 + (\Gamma/2)^2}$$

which shows a characteristic dip to (ideally) zero either above or below the peak, depending on the sign of $q$. The physics of the Fano resonance is the interference of alternative paths’ to the final outgoing energy state.

It is inherent in the “fuzzyness” of resonance peaks that they cannot be directly associated with standard isolated quantum-mechanical states. The resonance is a property of a whole surrounding of scattering states (associated with the Hamiltonian’s continuous spectrum), but no single state exhibits a priviledge role and the resonance nature truly only manifests itself by their phase relations, a rapid change of “scattering phases” as one passed the resonance energy.
The mathematical essence of the resonance is uncovered by entering the complex energy plane. A complex resonance energy

\[ W_r = E_r - i\Gamma/2 \]  

unites the resonance’s two key parameters. Being complex, this cannot be associated with the normal self-adjoint Hamiltonian. Historically, resonance energies where identified as position of poles found in the energy-dependent “scattering matrix” upon analytic continuation. If the poles are isolated (no other poles in a surrounding of radius \( \gtrsim \Gamma \)) and close to the real axis (small \( \Gamma \)), the Lorentzian peak results. It was also found that under suitable conditions the Hamiltonian itself can be analytically continued. The resulting non-Hermitian Hamiltonian can have the complex eigen energies \( W_r \) with square integrable functions associated with it, which fairly can be called a resonance state \( \Psi_r \), although this state has no strict interpretation in the framework of hermitian quantum mechanics. Reasoning from the complex plane requires analyticity properties, which we will discuss in some detail.

Taking the resonance state a face value, it decays at constant rate:

\[ ||\Psi_r(t)||^2 = ||e^{-itW_r/h}\Psi_r(0)||^2 = e^{-\Gamma t/\hbar}||\Psi_r(0)||^2 \]  

with a resonance “lifetime”

\[ \tau_r = \hbar/\Gamma. \]
The idea of decay at constant rate is used widely, although, strictly, there is little in standard quantum mechanics that supports it. It can be rigorously proven that at short times no quantum states can decay at constant rate (this is a rather simple, but beautiful consequence of assuming the time-evolution to be differentiable and reversible: as you start time-evolution either forward or backward in time must be the same, so the derivative of probability change must be 0). Less obviously, time-evolution cannot be exponentially decaying at long times, a fact that holds for any Schrödinger type Hamiltonian that has a ground state (a lower bound). Yet, at intermediate times one does find the near exponential decay associated with decay width $\Gamma$.

The underlying physics of resonances is more often than not the existence of an unperturbed Hamiltonian $H_0$ with a set of rigorous bound states that becomes coupled by an interaction $H_I$ to a continuum of some other Hamiltonian $H_C$ surrounding some of $H_0$’s bound states. In the simplest possible case we have the total Hamiltonian

$$H_0 + H_C + H_I = |\Phi_0\rangle E_0 \langle \Phi_0 | + \int dE |E\rangle \langle E | + |E\rangle c(E) \langle \Phi_0 | + |\Phi_0\rangle c^*(E) \langle E |$$

Due to the coupling $c(E)$ the bound state $\Phi_0$ “dissolves” into the continuum but it continues a ghost-like life in the complex plane and shapes the “density of states” of the continuum states associated with the real axis. The scattering states for that simple model can be written down in closed form and can be studied for insight into the nature resonances.

You may also recognize in the above the basic situation described by Fermi’s Golden Rule, which is nothing but approximation to $\Gamma$ for this case in second order perturbation theory.

1.8 Inverse scattering

By sending projectiles onto targets and watching the response, can we really expose the true nature of the target? Not usually. But sometimes the scattering problem can be inverted, i.e. we can reconstruct the scattering potential from complete knowledge of the scattering states. This so-called “inverse scattering” method has — to my knowledge — little application.
for the study of actual scattering processes. However, it is turns out to be a powerful method for constructing solutions to non-linear wave equations: the solutions appear as the reconstructed potentials for given (artificial) scattering data. Famous examples are the “non-linear Schrödinger equation” governing the formation of stable solitary waves in optical fibers,

\[ i \frac{d}{dt} A(x, t) = -\partial_x^2 A(x, t) + |A(x, t)|^2 A(x, t) \]  

(27)
or the non-linear “Korteweg-de-Vries” equation that describes the formation of unusually stable waves (“tidal bores”) running up rivers at from some shore lines:

\[ \frac{d}{dt} U(x, t) + 6U(x, t)\partial_x U(x, t) + \partial_x^3 U(x, t) = 0 \]  

(28)

Time permitting, we will touch upon this technique.

1.9 Scattering under time-dependent Hamiltonians

Finally I want to mention (and we will surely discuss it) the situation where we have a time-dependent Hamiltonian \( H(t) \). This usually results from modelling a physical system which can be, in part, described semiclassically. An important example is the interaction of quantum matter with intense laser light. Intense here means that absorption of a few photons by the microscopic target from the beam does not change the beam in any relevant amount. Another example is heavy ion scattering, where a not-so-heavy system just notices the rapidly changing Coulomb field of heavy ion passing with out the ion’s trajectory being significantly deflected.

For the laser case, at longer wave length, the Hamiltonian is reasonably described in dipole approximation

\[ H(t) = H_0 + \vec{E}(t) \cdot \vec{r}, \]  

(29)

where \( \vec{E}(t) \) the electric field of pulsed or also a continuous-wave (cw) laser. The time-dependent interaction leads to disintegration of an initially bound system. In the case of cw-lasers, the situation can be converted into a stationary problem and disintegration takes the form of a resonance decay into a “photon dressed” continuum. In case of finite pulse duration, techniques of standard scattering theory are applicable in principle, but often
the direct integration of the time-dependent Schrödinger equation is the
more feasible approach.

2 Non-relativistic quantum scattering theory

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 \( \mathbf{k}_i \) and \( \mathbf{q}_e \). This is what we
introduced as “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.

2.1 Mathematical modeling of a (simple) scattering experiment

Prepare a particle in some “free” state, e.g. free wave packet
\[
\Phi(\mathbf{r}, -t) = (2\pi)^{-3/2} \int d^{(3)}k e^{i\mathbf{k} \cdot \mathbf{r}} \psi(\mathbf{k})
\] (30)
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 ar-
  bitrary 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”)
2.2 The Möller operators

Now 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. Now we can 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:

\[ \lim_{t \to \pm \infty} U(-t)U_0(t) := \Omega_{\pm} \]  

(31)

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

\[ \exists T : \|U(t)U_0(-t) - \Omega_{\pm}\| < \epsilon, \quad \forall \pm t > T \]  

(32)

(“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 exist “pointwise” for any wave packet

\[ \|U(t)U_0(-t) - \Omega_{\pm}\| \Phi \rangle \to 0 \text{ for } \pm t \to \infty \]  

(33)

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

2.2.1 Properties

Note that the Möller operators map a wave-packet composed of free electrons (plane waves, \( \exp(i\vec{k}\vec{r}) \)) into a wave packet composed of scattering solutions \( \Psi_{\vec{k}}^{(\pm)}(\vec{r}) \) with asymptotic momenta \( \vec{k} \). We will find that the energies remain unchanged in the process (as it should be). We expect, in some sense,

\[ \Psi_{\vec{k}}^{(\pm)}(\vec{r}) = \Omega_{\pm} e^{i\vec{k}\vec{r}}. \]  

(34)

and

\[ -\frac{1}{2}\Delta e^{i\vec{k}\vec{r}} = H_0 e^{i\vec{k}\vec{r}} = \frac{\vec{k}^2}{2} e^{i\vec{k}\vec{r}} \quad \text{and} \quad (H_0 + V)\Psi_{\vec{k}}^{(\pm)} = H\Psi_{\vec{k}} = \frac{\vec{k}^2}{2}\Psi_{\vec{k}}. \]  

(35)

We say “in some sense”, as the involved waves are not in Hilbert space.
For the continuous spectrum we expect an intertwining property of the $\Omega_{\pm}$, i.e.

$$H\Omega_{\pm} = \Omega_{\pm}H_0.$$  \hspace{1cm} (36)

3 Hilbert space, operators, norms, spectrum

3.1 Operators

3.1.1 Domain

We first point out that any operator is only fully defined, if we specify also all functions from the Hilbert $\mathcal{H}$ space on which it is allowed to be applied, the domain $D(H) \subset \mathcal{H}$ of $H$. While everybody understands the necessity of excluding some functions from the domain, e.g. non-differentiable functions for differential operators, the domain is not, in general, defined uniquely in any natural fashion. It always has an element of a choice in it, which means that we really need to choose, which operator exactly we want to use, even if we already have fully defined it, say, for all functions of a countable basis. This choice ultimately determines such important properties as the spectrum of an operator (and whether it is real). The domain is an essential element of theory of unbounded operators and it is dealt with in functional analysis. It is not our ambition to dive into this other than mentioning that manipulating the domain can easily ruin the physically relevant properties of an operator.

3.1.2 Adjoint and self-adjoint operator

Given an operator $H$ and its domain $D(H)$, one can introduce the adjoint operator $H^\dagger$ and its domain $D(H^\dagger)$ through

$$D(H^\dagger) = \{ \phi \in \mathcal{H} | \sup_{\psi \in D(H)} \langle \phi | H\psi \rangle < \infty \}.$$ \hspace{1cm} (37)

Note that once $H$ and $D(H)$ are given, $D(H^\dagger)$ fully defined and there is no further element of choice. The action of $H^\dagger$ is then fully determined by defining all matrix elements

$$\phi \in D(H^\dagger), \psi \in D(H) : \langle H^\dagger \phi | \psi \rangle := \langle \phi | H\psi \rangle.$$ \hspace{1cm} (38)
In introductory quantum mechanics, the adjoint operator is introduced through Eq. (38) only, usually not discussing the domain of the adjoint. For (38) to provide a complete definition of the operator we need the completeness property of the Hilbert space and the continuity property of the scalar product $\langle \cdot | \cdot \rangle$. The domain (37) completes the definition of $H^\dagger$. The bottom line is: given $H$ and $D(H)$, its adjoint $H^\dagger$, $D(H^\dagger)$ is fully defined.

A self-adjoint (s.a.) operator is an operator

$$D(H) = D(H^\dagger), \quad H\psi = H^\dagger\psi, \quad \forall \psi \in D(H). \quad (39)$$

The term hermitian operator is limited in mathematics to operators

$$D(H) \subset D(H^\dagger), \quad H\psi = H^\dagger\psi, \quad \forall \psi \in D(H), \quad (40)$$

i.e. it does not guarantee the the operator and its adjoint have the same domain. This is a very important distinction, as only self-adjoint operators have strictly real spectrum, a property of great importance in physics.

3.1.3 Norm of an operator

We will need the “norm” of an operator, which can be introduced in several equivalent ways. We will mostly use the form

$$||H|| = \sup_{\psi \in D(H)} \frac{||H\psi||}{||\psi||} \quad (41)$$

An intuitive picture of the operator norm is the operator’s “largest eigenvalue”. Suppose the operator had a complete set of (possibly infinitely many) eigenvectors $\psi_n$ with eigenvalues $E_n$, then it is easy to see that this holds. We immediately see that an operator may (and in QM scattering theory often will) be unbounded, i.e. $||H|| = \infty$.

The intuition about the norm can be carried over to operators with continuous spectrum, where, instead of eigenfunctions, you imagine sequences of ever better concentrated wave-packets in the continuous spectrum.

Example: $\mathcal{H} = L^2(dx,[0,1])$, operator $(\hat{X}\phi)(x) = x\phi(x), D(\hat{X}) = \mathcal{H}$: $||\hat{X}|| = 1$. “Eigenfunctions” are $\delta$-function-like objects, that can be approximated by any sequence of “nice” functions $d_{x_0}(x)$ whose support increasingly concentrates around the spectral value $x_0$ (and whose norm are kept below some finite bound).
Problem 3.3: Operator norm  Let $A \in \mathcal{B}(\mathcal{H})$ be an operator with a complete set of eigenfunctions $|n\rangle$ for discrete eigenvalues $E_n$. Show that

$$||A|| = \sup_n |E_n|$$

Now let $X \in \mathcal{B}(\mathcal{L}^2(dx,[0,1]))$ be the operator

$$(X\phi)(x) = x\phi(x).$$

Clearly, this operator has purely continuous spectrum. Show that $||X|| = 1$.

Properties of the operator norm  The operator norm has all properties one expects of a norm

$$||P|| \geq 0 \quad \text{(42)}$$
$$||\alpha P|| = \alpha||P|| \quad \text{(43)}$$
$$||P|| = 0 \iff P = 0 \quad \text{(44)}$$
$$||P + Q|| \leq ||P + Q|| \quad \text{(45)}$$
$$||PQ|| \leq ||P|| ||Q|| \quad \text{(46)}$$

Also, it is compatible with the algebraic structure of (bounded) operators and with forming the adjoint, as follows:

$$||Q^\dagger|| = ||Q|| \quad \text{(48)}$$
$$||QQ^\dagger|| = ||Q|| ||Q^\dagger|| \quad \text{(49)}$$
$$||1|| = 1 \quad \text{(50)}$$

The bounded operators on a Hilbert space, denoted as $\mathcal{B}(\mathcal{H})$ form a Banach space, i.e. Cauchy-sequences have a limit that is also a bounded operator.

3.1.4 Limits for sequences of operators

Already for ordinary functions we know of different ways how a sequence can approach a limit (or fail to approach it). Let $f_n(x)$ be a sequence of
functions $\mathbb{R} \to \mathbb{R}$. If there is a function $f(x)$ such that
\[
|f_n(x) - f(x)| \to 0 \text{ for any } x \in \mathbb{R},
\] we say the function converges to $f$ point-wise. You have also met convergence w.r.t. to some $p$-norm on the function space $|| \cdot ||_p$, for example $L^2$ with $p = 2$ or $p = \infty$:
\[
||f||_\infty = \sup_x |f(x)|
\] meaning
\[
||f - f_n||_p \to 0
\] (52)
The difference between the function values is nowhere larger than $\epsilon$. In case of $|| \cdot ||_2$, the difference remain finite at a set of measure 0. For example, fourier series of discontinuous functions does not converge pointwise at the discontinuity, but the do converge for $p = 2$.

Similar distinctions are of special importance in scattering theory. Three different forms of convergence will be important:

**Norm-convergence**  $||H - H_n|| \to 0$ (similar to $p = \infty$ uniform convergence of functions). We also write
\[
\lim_{n \to \infty} H_n = H, \quad H_n \to H
\]

**Strong convergence**  $||(H - H_n)\psi|| \to 0$, $\forall \psi \in \mathcal{D}(H)$ (for simplicity consider only $\mathcal{D}(H) = \mathcal{D}(H_n)$). This is like point-wise convergence of a function. For strong convergence will write
\[
\lim_{n \to \infty} H_n = H, \quad H_n \to^s H
\]

**Weak convergence**  $\langle \chi | (H - H_n)\psi \rangle \to 0$, $\forall \chi, \psi \in \mathcal{D}(H)$, i.e. convergence of any legitimate matrix element. For weak convergence will write
\[
\lim_{n \to \infty} H_n = H, \quad H_n \to^w H
\]

On finite-dimensional spaces, all three kinds of convergence are equivalent.

The situation in scattering theory will be that the limit $t \to \infty$ will not exist in the norm, it will be trivially $=0$ in weak convergence, and only in strong ($\psi$-wise) convergence it will be what we really wish.
3.1.5 Stone’s theorem: Self-ajointness and unitarity

A unitary operator on a Hilbert space is defined as

\[ UU^\dagger = U^\dagger U = 1. \]  

(53)

This property also implies \( D(U) = \mathcal{H} \). Selfadjoint operators \( H \) and groups of unitary operators \( U(t) \) are intimately related by

**Theorem 1.** (Stone) Let \( U(t) \) be a strongly continuous one-parameter unitary group. Then it has the form \( U(t) = \exp(-itA) \) for some self-adjoint \( A \).

Here, “strongly continuous” means

\[ \lim_{h \to 0} ||U(h)\Psi - \Psi|| = 0, \]

(54)

i.e. the \( U(h) \) converges to \( 1 \) in the strong sense (“\( \Psi \)-wise”):

\[ \lim_{h \to 0} U(t + h) = U(t). \]

(55)

This is a theorem of central relevance for quantum mechanics: contrary to popular justifications for the preference of real-value spectra and “hermitian” operators, it is this relation between self-adjoint operators and unitary groups (symmetry transformations) that singles out the self-adjoint operators as the objects of choice in quantum mechanics.

3.1.6 Spectrum and resolvent

The mathematically solid way to define the spectrum is to consider its complement, the **resolvent set** \( \rho(H) \)

\[ \rho(H) = \mathbb{C}\setminus\sigma(H) = \{ z \in \mathbb{C} | \exists (H - z)^{-1}, ||(H - z)^{-1}|| < \infty \} \]

(56)

i.e. those \( z \) for which an inverse can be defined and has finite norm.

This reverts the pedestrian definition of spectral value

\[ \exists \psi_E : (H - E)\psi_E = 0, \]

(57)

which is difficult to make precise in Hilbert space as the continuous eigenfunctions are not from Hilbert space.
The set of operators labelled by $z$ ("operator-valued function")

$$R_H(z) := (H - z)^{-1}$$  \hspace{1cm} (58)

is called the **resolvent** of $H$. It is a bounded operator for all $z$ from the resolvent set. Its limit as $z$ approaches a spectral value plays a central role in scattering theory and goes by the name of "Green’s function" or "propagator".

This is often a much more pleasant object to deal with than the operator. For example, it is often analytic in $z$.

**Problem 3.4: Convergence of operators**  Let $\mathcal{B}(\mathcal{H})$ denote the space of bounded operators on a finite-dimensional Hilbert space $\mathcal{H}$ and let $\{B_n\}$ denote a sequence of operators. Show that the three following definitions of convergence are equivalent

1. Norm-convergence: $B_n \to B$ $\iff$ $\|B_n - B\| \to 0$ (Remember: $\|B\| = \sup_{\|\psi\|=1} \|B\psi\|$)
2. "Strong" convergence: $B_n \xrightarrow{s} B$ $\iff$ $\|B_n\psi - B\psi\| \to 0 \forall \psi \in \mathcal{H}$
3. "Weak" convergence: $B_n \xrightarrow{w} B$ $\iff$ $\langle \phi | (B_n - B)\psi \rangle \to 0 \forall \phi, \psi \in \mathcal{H}$

On infinite-dimensional Hilbert spaces this is not the case, there is only the implication norm-convergence $\Rightarrow$ strong convergence $\Rightarrow$ weak convergence.

(a) Using $\mathcal{H} = l^2$, i.e. the space of infinite length vectors, construct $B_n \xrightarrow{s} B$, but $B_n \not\to B$

(b) Construct $B_n \xrightarrow{w} B$, but $B_n \not\to B$.

**Hint:** In both cases the trick is to let escape the maps $B_n$ to ever new directions, e.g. by a sequence of operators that connect ever new pairs of entries etc.

**Problem 3.5: Resolvent**  Let $A \in \mathcal{B}(\mathcal{H})$ be a bounded operator on Hilbert space.
(a) Show that the formal series expansion

\[ (z - A)^{-1} = z^{-1} \sum_{n} (A z^{-1})^{n} \]

converges for \(|z| > ||A||\).

**Hint:** Use the properties of the operator norm to show the the series of finite sums is Cauchy.

(b) Conclude from the above that \((A - z)^{-1} \in \mathcal{B}(\mathcal{H})\) for \(||A|| < |z|\).

### 3.1.7 Spectral representation of self-adjoint operators

One very convenient property of self-adjoint operators is that they have a **spectral representation**. (Hermitian, but not s.a. operators, btw, do not necessarily have such a representation, this one reason why the distinction is important.) This is what you constantly use in quantum mechanics when you write things like

\[ H = \sum \int dE |E\rangle \langle E| = \sum_{n} |E_{n}\rangle E_{n} \langle E_{n}| + \int dE |E\rangle \langle E|, \]

where the \(|E\rangle\) are eigenfunctions

\[ H|E\rangle = |E\rangle E \]

with the normalization

\[ \langle E_{n}|E_{m}\rangle = \delta_{mn} \text{ for bound states, } \langle E|E'\rangle = \delta(E - E') \text{ for continous states.} \]

Self-adjointness is a sufficient, but not necessary condition for the existence of a spectral representation. In fact, all operators that are bounded and **normal** do have a spectral representation. Normal means here that the operator commutes with its adjoint:

\[ H^{\dagger} H = HH^{\dagger}. \]

(For unbounded operator, this definition of “normal” must be modified.)

One such case is the unitary time-evolution operator of quantum mechanics

\[ U(t) = \exp(-itH), \]
which we can write as

$$U(t) = \sum dE |E\rangle \exp(-itE) \langle E|.$$  \hfill (65)

The spectral representation is extremely useful as it allows to think of a self-adjoint operator pretty much like of a multiplication by the spectral values. Operators that have a spectral representation and sets of such operators that commute are indeed closely related to ordinary functions, where formation of the adjoint maps into taking the complex conjugate.

A somewhat more rigorous statement of the spectral theorem uses the fact that there exists an $L^2$ Hilbert space on the spectrum of $H$

$$\mathcal{H}_\sigma = L^2(\mu(E), \sigma(H)),$$  \hfill (66)

where $\mu(E)$ is a measure on the real axis, which is the Lebesgue measure for the continuous spectrum (usual integration) and the $\delta$-like Dirac measure for the “point spectrum” of bound state energies. The spectral theorem than says that there exists a unitary map from the spectral space to the original Hilbert space

$$U_H : \mathcal{H}_\sigma \to \mathcal{H} : |\phi_\sigma\rangle \to |\phi\rangle = U_H |\phi_\sigma\rangle,$$  \hfill (67)

by which we bring the operator $H$ to diagonal (multiplication-by-eigenvalue) form

$$H = UdHU^{-1} : (d_H\phi_\sigma)(E) = \phi_\sigma(E)E.$$  \hfill (68)

Unitarity is here to be understood as $||U\phi_\sigma||_{\mathcal{H}_\sigma} = ||\phi||_{\mathcal{H}}$

### 3.1.8 Fourier transform

The one-dimensional spectral representation of $i\partial_x$, $\mathcal{H}_\sigma = L^2(dk, \mathbb{R})$

$$U_{i\partial_x} = F(\phi)(k) = (2\pi)^{-1/2} \int_{-\infty}^{\infty} e^{ikx}\phi(x)dx$$  \hfill (69)

Unitarity = Parseval

### 3.1.9 Degeneracy

Label eigenvectors in a degenerate subspace by $\alpha$: may be a discrete index like, say $l, m$ of angular momentum, or a continuous index, say, if you
consider the operator $-\partial^2_x$ in $L^2(dx dy | \mathbb{R}^2)$ where $\alpha = y$,

$$H = \sum \! \! \! \! \int d\alpha \int dE |E, \alpha \rangle \langle E, \alpha|.$$  \hfill (70)

A whole (finite or infinite) set of functions is associated with each $E$. In case of the point spectrum this is a subspace of $\mathcal{H}$.

**Problem 3.6: Spectral representation**  Make the final steps to get the spectral representation of $U(t)$.

**Problem 3.7: Spectral representation**  Write the spectral representation of $-\Delta$ as defined in the lecture, using $lm$ for labelling the degeneracy.

**Hint:** Use the following expansion

$$e^{i\vec{k} \cdot \vec{r}} = \sum_{lm} Y^m_l(\hat{k}) Y^m_l(\hat{r}) j_l(kr),$$  \hfill (71)

where $j_l$ are the spherical Bessel functions.

3.1.10 Functions of operators

The spectral representation is also a standard way for defining functions of operators

$$f(H) = \sum \! \! \! \! \int dE |E\rangle f(E) \langle E|.$$  \hfill (72)

This works for any function, be it $\exp(itE)$ for the exponential, or for the characteristic function

$$\chi(H) = \sum \! \! \! \! \int dE |E\rangle \chi_{[a,b]}(E) \langle E|.$$  \hfill (73)

which is a projector onto a spectral subspace. We will even write things like

$$\delta(H - E_0) = \sum \! \! \! \! \int dE |E\rangle \delta(E - E_0) \langle E| = |E_0\rangle \langle E_0|$$  \hfill (74)

to express a “projector” onto scattering eigenfunctions. (This will not be an operator in Hilbert space!). Computation rules work fine, the meaning, where we will be using this, can be made precise in the mathematical sense, but we will usually rely on the expression’s formal appeal.
3.2 Spectral properties and dynamical behavior

In physics we like to think of bound states - that never seriously leave some finite region, and unbound states, that are certain to leave any finite surrounding of the system. We also have got accustomed to associating these two types of states with discrete and continuous spectrum, respectively. Not much of a justification is given for this usually. We will first establish that fact rigorously. The main theorem expressing this fact is called RAGE (for Ruelle, Amrein, Georgescu, Enß).

3.2.1 Spectral subspaces

A general theorem of measure theory (Lebesgues decomposition theorem) implies that the spectrum can be separated into point, absolutely continuous, and singular spectrum

\[ \langle \phi | dP(\lambda) \psi \rangle = d\mu_{\phi,\psi} + d\mu_{ac;\phi,\psi} + d\mu_{\text{sing};\phi,\psi}, \]

(75)
each associated with a subspace of the Hilbert space. These subspaces are mutually orthogonal spaces

\[ \mathcal{H} = \mathcal{H}_p \oplus \mathcal{H}_{ac} \oplus \mathcal{H}_{\text{sing}} =: \mathcal{H}_p \oplus \mathcal{H}_c. \]

(76)

We have lumped singular and ac into “continuous” \( \mathcal{H}_c \), as these two parts behave similar in many respects and actually, usual Schrödinger operators have empty singular spectrum. There we will assume that our operators have no singular spectrum (this is proven for large classes of Schrödinger type operators, especially for the short range potentials considered in scattering theory. We may also write

\[ \mathcal{H}_p = \text{span}(\text{eigenvectors}) \]

(77)

and

\[ \mathcal{H}_c = \mathcal{H}_p^\perp \]

(78)

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

\[ \lim_{t \to \pm \infty} \langle e^{-itH} \psi | \phi \rangle = 0, \]

(79)

we can say: after long time, the wave packet becomes orthogonal to any fixed state. This is at completely generic property of the ac spectral sub-
space. We know it as wave-packed spreading in QM. It is related to the ac spectrum of $\Delta$.

For functions from the sing 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 sing 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.

3.2.2 Fourier transform of smooth functions (Riemann-Lebesgue)

We had discussed the absolutely continuous measures as those that are equivalent to the Lebesgue measure in the sense $d\mu_{ac}(x) = f(x)dx$ with an integrable function $f$. That means that for the absolutely continuous part of the spectral measure we can take advantage of the following

**Theorem 2.** (Riemann-Lebesgue) If Lebesgue integral of $|f|$ is finite, then the Fourier transform of $f$ satisfies

$$\hat{f}(\lambda) := \int_{\mathbb{R}} f(x) \exp(-i\lambda x) \, dx \to 0 \text{ as } |\lambda| \to \infty.$$ 

We leave this important and useful theorem without proof. It makes precise our intuition that a highly oscillatory integral ($|z| \to \infty$) will eventually average to zero, if the integrand is otherwise “smooth”, i.e. without non-integrable singularities.

3.3 Classes of operators

We have met hermitian, self-adjoint, and unitary operators, we have distinguished bound and undbound a operators by their norms. Operators can be classified by many other criteria. A few of them are particularly important.
3.3.1 (Orthogonal) projectors

3.3.2 Compact operators

3.3.3 Relatively bounded operators

In scattering theory it is important, how one operator relates to another, e.g. $H_0$ to $V$, how “big” $V$ is compared to $H_0$. An well known example is the fact that reasonable Hamiltonians should have a lower bound, if a potential is added to kinetic energy. $V$ being not too big compared to $H_0$ could be expressed as $\|V/H_0\| < \infty$. The problem, that $H_0$ may be singular is circumvented by using the resolvent instead.

**Definition 1.** Let $V$, $H$, $D(V) \subset D(H)$. If

$$\|V(H - z)^{-1}\| < \infty, \text{ for some } z \in \rho(H)$$

we call $V$ relatively bounded w.r.t. $H$.

Under these conditions, perturbation of $H + \alpha V$ theory will be convergent. (The condition is NOT fulfilled for popular perturbers such as in the Stark effect, for who the perturbations series does actually NOT converge).

3.3.4 Relatively compact operators

Analogously

**Definition 2.** Let $V$, $H$, $D(V) \subset D(H)$. If

$$V(H - z)^{-1} \text{ for some } z \in \rho(H)$$

is compact we call $V$ relatively compact w.r.t. $H$.

Relatively compact operators play an important role in scattering theory. Relative compactness expresses, in a mathematically precise manner, that $H + V$ differs from $H$ significantly (more than any given $\epsilon$) only on a finite subspace. As a wavepacket spreads, it looses its overlap with any such finite subspace and its dynamics differs by arbitrarily little from a free wave packet.

3.3.5 The RAGE theorem

This theorem by named after Ruelle, Amrein, Georgescu, and Enß states that there is a strict relation between point spectrum and continuous
spectrum of an operator $H$ on the one hand and the long-time evolution $\exp(-itH)$ of functions from the corresponding subspaces $\mathcal{H}_p$ and $\mathcal{H}_c$, as we would expect it: in the long run, functions from $\mathcal{H}_p$ will remain within a “finite” region of the Hilbert space (although that region may need to be large), while functions from $\mathcal{H}_c$ will, in the long run, leave any “finite” region of the Hilbert space. There is a one-to-one relation between the spectral properties and the long-time behavior of the dynamics.

Relative compactness allows us to single out a “finite” subspace of 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.

This theorem allows us to formulate the following theorem, that tells us that time-evolution separates the (at least on average) the Hilbert space into parts that leave any finite subspace and parts that will remain contained in a finite subspace.

**Theorem 3. (RAGE).** Let $A$ be self-adjoint. Suppose there is a sequence of relatively compact operators $K_n$ which converges strongly to identity. Then

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

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 $K_n$ 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 point spectrum: spectral properties and time-evolution behavior match one-to-one.

**check** for ac the time-average can be replaced by time-limits

30
3.3.6 Asymptotic completeness

We already discussed that $\Omega_\pm$ will not in general be unitary as maps $\mathcal{H} \to \mathcal{H}$. At finite times $t$ the operator $U(t)U_0(-t)$ is unitary. 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 as maps on $\mathcal{H}$, 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 $H_0 = -\Delta$: $P_{ac}(H_0)\mathcal{H} = \mathcal{H}$. 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 and that the dynamics of the unbound (ac) states of the the two systems are equivalent: 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).

3.3.7 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. $||V(-\Delta + 1)^{-1}|| < \infty$. Note that, as $\sigma(-\Delta) = \mathbb{R}_+$ is positive, we can use the a real offset instead of the complex $z$ for the general self-adjoint case.

A relatively bounded perturbation $V$ of the Laplacian $-\Delta$ is called short
range if
\[ \int_0^\infty ||V(-\Delta + 1)^{-1}1_{\mathbb{R}^3 \setminus B_r}||dr < \infty \] (80)
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: remember that 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.

**Problem 3.8:** \( r^{-1-\epsilon} \) is short range  Proof this.
**Hint:** Fourier transform is... 

**Theorem 4.** (Volker Enß) Suppose \( V \) is short range. Then the Møller operators exist and are asymptotically complete.

**Examples** Potentials behaving asymptotically as \( r^{-1+\epsilon} \) are short range for any \( \epsilon > 0 \). This leaves the Coulomb potential as the only relevant violator in situations where we want to talk about “scattering” at al.

**Problem 3.9:** Relative boundedness Show that the Coulomb potential is bounded relative to \(-\Delta\). Show that the Coulomb potential is not short range.

Technically, the short range property is mostly exploited in the form of the compactness of
\[ (H - z)^{-1} - (H_0 - z)^{-1} \quad \text{and} \quad f(H) - f(H_0) \] (81)

**Lemma 1.** If \( V \) is short range, then \( R_H(z) - R_{H_0}(z) \) is compact.

For the proof of the lemma we would need a few results on compactness that we have skipped. However, it gives some insight to consider the ideas of the proof

- Denote \( \chi_r(x) = \chi_{\{x||x|>r\}}(x) \), the projector onto the remote parts of space
- So, \( 1 - \chi_r \) projects onto a finite range.
We use the \((1 - \chi_r)R_{H_0}(z)\) is compact (without proof). In fact, the product of any two operators \(g(x)f(p)\) for integrable functions \(g, f\) that decay to 0 at large \(x\) and \(p\) turns out to be compact (Teschl 7.21).

Also, \(R_H(z)V\) is bounded: that is plausible, as \(R_{H_0}(z)\) is bounded and 
\(H = H_0 + V\), closely related to Kato-Rellich. (Proof in Teschl 6.23).

Now the short range condition enters
\[
\lim_{r \to \infty} R_H(z)V(1 - \chi_r)R_{H_0}(z) \to R_H(z)VR_{H_0}(z)
\]

Note the identity
\[
R_H(z)VR_{H_0}(z) = (H_0 + V - z)^{-1}V(H_0 - z)^{-1} = (H_0 + V - z)^{-1} - (H_0 - z)^{-1}
\]

Actually, short range implies that for any function that decays at \(\infty\), we have

**Lemma 2.** Suppose \(R_H(z) - R_{H_0}(z)\) is compact. Then so is \(f(H) - f(H_0)\) for any \(f \in C_\infty(\mathbb{R})\) and
\[
\lim_{r \to \infty} \|[f(H) - f(H_0)]\chi_r\| = 0. \tag{82}
\]

**Proof.** Again the proof involves technical results that were skipped (Teschl 6.21). But once we know that \(f(H) - f(H_0)\) is compact, we know that \(\chi_r\) excludes an arbitrarily large space, i.e. any \(\chi_r \phi\) goes strongly to zero. Multiplying by a compact operator does not change that. As the family of maps is bounded and goes to zero strongly, it goes to zero uniformly, i.e. in the operator norm.

3.3.8 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).

3.3.9 The S-matrix

3.4 Problems

3.4.1 $\delta$-Function of a self-adjoint operator

3.4.2 Abel formula

Problem 3.10: Abel limit

(a) Convince yourself of the Abel-limit:

\[
f(t) \to f_\infty \quad \Rightarrow \quad \lim_{\epsilon \downarrow 0} \epsilon \int_0^\infty e^{-t\epsilon} f(t) dt = f_\infty
\]

(b) Show the same for the strong limit:

\[
V(t) \xrightarrow{\text{s}} V_\infty \quad \Rightarrow \quad \text{s-lim}_{\epsilon \downarrow 0} \epsilon \int_0^\infty e^{-t\epsilon} V(t) dt = V_\infty.
\]

4 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.

4.1 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” $H_k^{\pm} = \frac{k^2}{2} \Psi_k^{\pm}$. 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 wave free wave packet $\varphi_{\vec{k}} \sim e^{i\vec{k} \cdot \vec{r}}$, then

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

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 $\Psi_{\vec{k}}$. Conversely, the “out”-states $\Psi^{(-)}$ are like plane waves in the remote future. Note that in physics literature, the sign convention of $\Psi^{(\pm)}$ is often reverted, the signs relating to the $\epsilon$-limits to be discussed below. We will adhere to the more physical concept of associating + with conditions at large positive times.

The similarity to the LS equation becomes even more evocative, when we will show that in the spectral representation of $H_0$ we have

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

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 difficult to use in computations, to put it mildly. (Time permitting, we may introduce techniques that allow the direct numerical evaluation of such expressions.) But it can be transformed to the LS equation.

4.2 $\Omega_{\pm}$ in the spectral representation of $H_0$

$\Omega_{\pm}$ are time-independent 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

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

(85)
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).

In the spectral representation of $H_0$

$$H_0 = \int_0^\infty E dP(E)$$  \hspace{1cm} (86)

we write

$$e^{itH}e^{-itH_0} = e^{itH} \int_0^\infty e^{-itE} dP(E) = \int_0^\infty e^{it(H-E)} dP(E)$$  \hspace{1cm} (87)

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

$$\Omega_+ = \lim_{\epsilon \downarrow 0} \epsilon \int_0^\infty e^{-\epsilon t} \int_0^\infty e^{\pm it(H-E)} dP(E) dt$$ \hspace{1cm} (88)

$$= \lim_{\epsilon \downarrow 0} \epsilon \int_0^\infty \int_0^\infty e^{\pm it(H-E\pm i\epsilon)} dt dP(E)$$  \hspace{1cm} (89)

$$= \lim_{\epsilon \downarrow 0} \pm i\epsilon \int_0^\infty (H-E\pm i\epsilon)^{-1} dP(E)$$ \hspace{1cm} (90)

$$= 1 - \lim_{\epsilon \downarrow 0} \int_0^\infty (H-E\pm i\epsilon)^{-1} V dP(E)$$ \hspace{1cm} (91)

The last step is by some algebra with the resolvent

$$(H-E\pm i\epsilon)^{-1}(\pm i\epsilon) = (H-E\pm i\epsilon)^{-1}[(H-E\pm i\epsilon) - (H-E)]$$

$$= 1 - (H-E\pm i\epsilon)^{-1}(H_0 + V - E)$$ \hspace{1cm} (92)

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

$$H = \int G dP_H(G)$$ \hspace{1cm} (93)

for the projection valued measure $P_H$ belonging to $H$. Then

$$\int_0^\infty e^{\pm it(H-E\pm i\epsilon)} dt = \int \int_0^\infty e^{\pm it(G-E\pm i\epsilon)} dP(G) dt$$ \hspace{1cm} (94)
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

$$\Psi^{(\pm)} = \Omega_{\pm} \phi = \phi - \lim_{\epsilon \downarrow 0} \int_{0}^{\infty} (H - E \pm i\epsilon)^{-1} VdP(E) \phi, \quad (95)$$

which bears great similarity with the LS equation. Actually, it is seemingly better, 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.

Now we remember the symmetric role of $H$ and $H_0$ in scattering theory and we interchange them

$$H, H_0, H - H_0 =: V \rightarrow H' = H_0, H'_0 = H, H' - H'_0 = H_0 - H = -V \quad (96)$$

to write

$$\phi^{(\pm)} = \Psi + \lim_{\epsilon \downarrow 0} \int_{0}^{\infty} (H_0 - E \pm i\epsilon)^{-1} VdP_H(E)\psi, \quad \psi \in P_{ac}(H)H. \quad (97)$$

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

$$\Psi^{(\pm)} = \phi - \lim_{\epsilon \downarrow 0} \int_{0}^{\infty} (H_0 - E \pm i\epsilon)^{-1} VdP_H(E)\Psi^{(\pm)}. \quad (98)$$

**Problem 4.11:** Directly derive the Lippmann-Schwinger equation  

We had used that on $H_{ac}$ one can interchange $H_0 \leftrightarrow H$ to obtain the Lippmann-Schwinger equation from the definition of the Møller operators. Alternatively one can form the inverses $\Omega_{\pm}^{-1}$ to arrive at the same result. Do that.

**Hint:** Show by simple algebraic manipulations

$$1 - (H - z)^{-1}V = [1 + (H_0 - z)^{-1}V]^{-1}$$

4.2.1 Remark on “$ac$-spectral eigenfunctions”

The equation above is almost the shape of the LS equation. However, it is formulated for wave-packets rather than, as physicists like to do it,
for “eigenfunctions of the continuous spectrum”. For $-\Delta$ these would be plane waves $\exp(ik \cdot x)$. Indeed, the path for making this notion precise, is through the Fourier transform and using the mapping by $\Omega_\pm$, formally
\[
|\vec{k}\rangle^{(\pm)}_H = \Omega_\pm |\vec{k}\rangle_{H_0} := \Omega_\pm e^{i\vec{k} \cdot \vec{x}}.
\] (99)

The mapping is not unique because of the two alternative signs, but it does not need to be, as the energies are degenerate and any linear combination is a possible choice. The asymptotic condition of matching either in the future or in the past fixes the basis in this degenerate subspace. Time-reversal maps between the two signs. Accepting that, we can even give meaning to the $\delta$-function of the Hamiltonian as the spectral projector onto the eigenfunctions of given energy
\[
\int_0^\infty \delta(H - E) dE := \int dk \int d\alpha \frac{k}{2} |k, \alpha\rangle \langle k, \alpha|
\] (100)
\[
= \int_0^\infty dE \int d\alpha \frac{E^{1/2}}{2} |\sqrt{E}, \alpha\rangle \langle \sqrt{E}, \alpha|
\] (101)
\[
= \int_0^\infty dE \int d\alpha |\tilde{E}, \alpha\rangle \langle \tilde{E}, \alpha|
\] (102)
where
\[
|\tilde{E}, \alpha\rangle = \frac{E^{1/4}}{\sqrt{2}} |\sqrt{E}, \alpha\rangle.
\] (103)

If we do that, formally, the $\delta(H - E)$ allows to perform the $dE$ integration and we have the Lippmann-Schwinger equation for the scattering solutions
\[
\Psi^{(\pm)}(E) = \phi(E) - \lim_{\epsilon \downarrow 0} (H_0 - E \pm i\epsilon)^{-1} V \psi^{(\pm)}(E).
\] (104)
where the $+$ corresponds to matching of asymptotics of $\phi = e^{i\vec{k} \cdot \vec{r}}$ in the remote future and $-$ to matching in the remote past.

4.3 Mapping free to free spaces: the $S$-matrix

With asymptotic completeness the $\Omega_\pm$ are unitary bijections $P_{ac}(H)\mathcal{H} \leftrightarrow P_{ac}(H_0)\mathcal{H}$ and the $S$-matrix maps $P_{ac}(H_0)\mathcal{H} \rightarrow P_{ac}(H_0)\mathcal{H}$
\[
S = (\Omega_+)^{-1} \Omega_- = \Omega_+^* \Omega_-
\] (105)
This corresponds to a limit
\[
\lim_{t \to \infty} [U(-t)U_0(t)]^{-1}[U(t)U_0(-t)] = \lim_{t \to \infty} U_0(-t)U(2t)U_0(-t) \tag{106}
\]
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 properties of the $S$-matrix:
- is unitary (asymptotic completeness)
- it “inherits” symmetries from $H$ and $H_0$.
- it conserves energy - intertwining relation

### 4.3.1 Spectral representation of the $S$-matrix

In the same spirit as for $\Omega_{\pm}$, there is a representation of the $S$-matrix in the spectral representation of $H_0$:

\[
S = \lim_{\epsilon \downarrow 0} \int_0^\infty dE \left\{ 1 - 2\pi i \delta(H_0 - E) \left[ V - V(H - E - i\epsilon)^{-1}V \right] \right\} \delta(H_0 - E). \tag{107}
\]

We use the (only slightly) symbolic notation
\[
\delta(H_0 - E) = \sum_{\alpha} |E, \alpha \rangle \langle E, \alpha|, \tag{108}
\]
where $\alpha$ labels the degeneracy in the energy subspace $E$.

#### Derivation of the $S$-matrix

\[
S = s\lim_{\epsilon \downarrow 0} \epsilon \int_0^\infty dt \int_0^\infty \int_0^\infty dE dE' \delta(H_0 - E)e^{-it\left(H - \frac{E + E'}{2} - i\epsilon \right) - i\epsilon} \delta(H_0 - E')
\]
\[
= s\lim_{\epsilon \downarrow 0} \epsilon \int_0^\infty dt \int_0^\infty \int_0^\infty dE dE' \delta(H_0 - E) \frac{-i\epsilon}{H - \frac{E + E'}{2} - i\epsilon} \delta(H_0 - E')
\]

**Problem 4.12: Resolvent equation** An important identity for $H = H_0 + V$:
\[
(H - z)^{-1} = (H_0 - z)^{-1} - (H_0 - z)^{-1}[V - V(H - z)^{-1}V](H_0 - z)^{-1} \tag{109}
\]
Verify this!

The first term evaluates to

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

(110)

Further

Problem 4.13: $\delta$-function

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

(111)

By this, one can integrate over $E'$ for the second term and one arrives at Eq. (107).

4.3.2 The $T$-matrix

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

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

(112)

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

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

(113)

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

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

(114)

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

$t(\vec{k}, \vec{k}')$ contains the relevant scattering information. Also, it is a smooth function of $\vec{k}, \vec{k}'$, loosely speaking, where solutions of the LS equation exist. It essentially is the same as the scattering amplitude $f(k, \vec{n}, \vec{n}')$

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

(115)

whose square gives the differential cross section:

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

(116)
Problem 4.14: δ-function  

The δ-“function” is fully defined by its property

\[ \int dx \delta(x) g(x) = g(0) \quad \forall g \in C_0^\infty, \]  

(117)

(Here, \( C_0^\infty \) designates the infinitely differentiable functions with compact support.) Remind yourself of the following properties of the δ-function and show them using Eq. (117):

(a) Let \( f_\epsilon, \int_\mathbb{R} f_\epsilon(x)dx = 1 \) be a family of functions such that \( \lim_{\epsilon \downarrow 0} \int_{-\epsilon}^{\epsilon} f_\epsilon(x) = 1 \). Show \( f_\epsilon \rightarrow \delta(x) \).

(b) \( \lim_{\epsilon \downarrow 0} \Im m \frac{1}{x-x_0-i\epsilon} = \pi \delta(x-x_0) \)

(c) \[ \delta(ax) = \frac{\delta(x)}{|a|} \]

\[ \delta\left(\frac{k'^2}{2} - \frac{k''^2}{2}\right)\delta(k'_x - k''_x)\delta(k'_y - k''_y) = \delta(3)(\vec{k}' - \vec{k}'')/k'_z \]

4.4 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 $\phi(\vec{k}) \rightarrow \phi(\vec{k}) e^{i\vec{a}\cdot\vec{k}}$. Remember that multiplication by $e^{i\vec{a}\cdot\vec{p}}$ in $\vec{p}$-space is equivalent to applying the shift-operator $\exp(i\vec{a}\cdot\vec{p})$ in $\vec{x}$-space. The scattered shifted wave packet is

$$\psi_{\vec{a}} = S \phi_{\vec{a}}. \quad (118)$$

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 $\Delta k$ is

$$\int_{\Delta\Omega} d\Omega \int_{\Delta k} dk k^2 |\psi_{\vec{a}}(\vec{k})|^2 \quad (119)$$

Here we use polar coordinates $k, \theta, \phi$:

$$\vec{k} = k \begin{pmatrix} \sin \theta \cos \phi \\ \sin \theta \sin \phi \\ \cos \theta \end{pmatrix} \quad (120)$$

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

$$\int_{\Delta\Omega} d\Omega \int_{\Delta k} dk = \int_{\theta_1 - \Delta\theta}^{\theta_1 + \Delta\theta} d\theta \sin \theta \int_{\phi_1 - \Delta\phi}^{\phi_1 + \Delta\phi} d\phi \int_{k_1 - \Delta k}^{k_1 + \Delta k} dk \quad (121)$$

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

$$\frac{1}{A} \int_A d^2 a \int_{\Delta\Omega} d\Omega \int_{\Delta k} dk k^2 |\psi_{\vec{a}}(\vec{k})|^2 \quad (122)$$
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 (107) does not give a contribution. The cross section is

$$\sigma(\vec{k}, \vec{k}') := \int_A d^{(2)}a \int_{\Delta \Omega} d\Omega \int_{\Delta k} dk k^2 |\psi_\alpha(\vec{k})|^2$$

$$= \int_A d^{(2)}a \int_{\Delta \Omega} d\Omega \int_{\Delta k} dk k^2 \left| \int d^{(3)}k' \int dE' \delta(\frac{k^2}{2} - E')t(\vec{k}, \vec{k}')\delta(\frac{k'^2}{2} - E')\phi(\vec{k}')e^{i\vec{a}\vec{k}'} \right|^2$$

where we have defined

$$t(\vec{k}, \vec{k}') = 2\pi \langle \vec{k}|V - V(H - k^2/2 - ie)^{-1}V|\vec{k}' \rangle. \quad (123)$$

This becomes

$$= \int_A d^{(2)}a \int_{\Delta \Omega} d\Omega \int_{\Delta k} dk k^2 \int d^{(3)}k' \int dE' \int d^{(3)}k'' \int dE'' \quad (124)$$

$$\delta(\frac{k^2}{2} - E')\delta(\frac{k'^2}{2} - E')\delta(\frac{k''^2}{2} - E'')\delta(\frac{k'^2}{2} - E'') \quad (125)$$

$$t^*(\vec{k}, \vec{k}')t(\vec{k}, \vec{k}'')\phi^*_\alpha(\vec{k}')(\vec{k})\phi^*_\alpha(\vec{k}'')e^{i\vec{a}(\vec{k}'' - \vec{k}')} \quad (126)$$

Integration over $E'$ and $E''$ leads to

$$= \int_A d^{(2)}a \int_{\Delta \Omega} d\Omega \int_{\Delta k} dk k^2 \int d^{(3)}k' \int d^{(3)}k'' \quad (127)$$

$$\delta(\frac{k^2}{2} - \frac{k'^2}{2})\delta(\frac{k^2}{2} - \frac{k''^2}{2})t^*(\vec{k}, \vec{k}')t(\vec{k}, \vec{k}'')\phi^*_\alpha(\vec{k}')(\vec{k})\phi^*_\alpha(\vec{k}'')e^{i\vec{a}(\vec{k}'' - \vec{k}')} \quad (128)$$

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

$$= \int_A d^{(2)}a \int_{\Delta \Omega} d\Omega k \int d^{(3)}k' \int d^{(3)}k'' \quad (129)$$

$$\delta(\frac{k'^2}{2} - \frac{k''^2}{2})t^*(\vec{k}, \vec{k}')t(\vec{k}, \vec{k}'')\phi^*_\alpha(\vec{k}')(\vec{k})\phi^*_\alpha(\vec{k}'')e^{i\vec{a}(\vec{k}'' - \vec{k}')} \quad (130)$$
For the integral over \(d^{(2)}a\) we observe that
\[
\int_A d^{(2)}ae^{i\vec{a}((\vec{k}''-\vec{k}'))} = (2\pi)^2\delta(k_x'^' - k_x'')\delta(k_y'^' - k_y''')
\] (131)
and obtain
\[
= (2\pi)^2 \int_{\Delta\Omega} d\Omega k \int d^{(3)}k' \int d^{(3)}k''
\delta(\frac{k'^2}{2} - \frac{k''^2}{2})\delta(k_x'^' - k_x'')\delta(k_y'^' - k_y''') = \delta^{(3)}(\vec{k}'' - k_z'')/k_z'
\] (132)
The three 1-dimensional deltas combine to
\[
\delta(\frac{k'^2}{2} - \frac{k''^2}{2})\delta(k_x'^' - k_x'')\delta(k_y'^' - k_y'''') = \delta^{(3)}(\vec{k}'' - k_z'')/k_z'
\] (133)
and another integral goes away
\[
= (2\pi)^2 \int_{\Delta\Omega} d\Omega \int d^{(3)}k' |t(\vec{k}, \vec{k}')|^2 |\phi_{\vec{a}}(\vec{k}')|^2 \frac{k_z'}{k_z}
\] (134)
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 \(||\phi|| = 1\)
\[
= (2\pi)^2 \int_{\Delta\Omega} d\Omega |t(\vec{k}, \vec{k}_0)|^2
\] (135)
To connect to conventional notation, we introduce the
**Scattering amplitude**
\[
f(\vec{k}, \vec{k}_0) := -(2\pi)t(\vec{k}, \vec{k}_0) = -(2\pi)^2\langle\vec{k}|V - V(H - k^2/2 - i\epsilon)^{-1}V|\vec{k}_0\rangle
\] (136)
and write the **scattering cross section**
\[
\frac{d\sigma(\vec{k}, \vec{k}_0)}{d\Omega} = |f(\vec{k}, \vec{k}_0)|^2
\] (137)
If our \(H_0\) is the free time-evolution with the \(\delta\)-normalized scattering functions \(|\vec{k}\rangle = e^{i\vec{k}\vec{x}}/(2\pi)^{3/2}\), the scattering amplitude is expressed in terms of the plane wave matrix elements
\[
f(\vec{k}, \vec{k}_0) = -(2\pi)^{-1}\langle e^{i\vec{k}\vec{x}}|V - V(H - k^2/2 - i\epsilon)^{-1}V|e^{i\vec{k}_0\vec{x}}\rangle
\] (138)
Post- and prior forms: Using the Møller operator equation in the form
\[
\Psi^{(\pm)}(\vec{k}) = \Omega_{\pm} |\vec{k}\rangle = \left[ 1 - (H - k^2/2 \pm i\epsilon)^{-1} V \right] |\vec{k}\rangle \tag{140}
\]
the scattering amplitude can also be written as
\[
f(\vec{k}, \vec{k}_0) = -(2\pi)^2 \langle \vec{k} | V | \Psi^{(-)}(\vec{k}) \rangle \quad \text{“post” form} \tag{141}
\]
\[
= -(2\pi)^2 \langle \Psi^{(+)}(\vec{k}) | V | \vec{k}_0 \rangle \quad \text{“prior” form} \tag{142}
\]
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.
\[
\langle \Psi^{(+)}(\vec{k}) | V | \vec{k}_0 \rangle = \langle \Omega_+ \vec{k} | V | \vec{k}_0 \rangle = \langle \vec{k} | \Omega_+ V | \vec{k}_0 \rangle = \langle \vec{k} | [1 - (H - k^2/2 + i\epsilon)V] V | \vec{k}_0 \rangle = \langle \vec{k} | [1 - V (H - k^2/2 - i\epsilon)] V | \vec{k}_0 \rangle.
\]
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 \(\Omega\)
\[
\sigma_{tot} = \int d\Omega |f(k, \Omega, \Omega_0)|^2 \tag{143}
\]

4.4.1 The LS equation in position space

The important point of the LS-equation is that the Green’s function of free motion \((H_0 - E \mp i\epsilon)^{-1}\) can be evaluated explicitly (in stark contrast to the full Green’s function). In position space, the LS equation takes the form
\[
\Psi^{(\pm)}(\vec{r}) = e^{i\vec{k}\vec{r}} - \int_{\mathbb{R}^3} e^{\mp i\vec{k}|\vec{r} - \vec{r}'|} \frac{1}{4\pi |\vec{r} - \vec{r}'|} V(\vec{r}') \Psi^{(\pm)}(\vec{r}'). \tag{144}
\]
where we recognize the form of the solution \(\Psi^{(\pm)}(\vec{r})\) as a plane wave plus a superposition of spherical waves.
Problem 4.15: Green’s function in position space

Compute the function

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

(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.

### 4.5 Asymptotic behavior

Asymptotically, i.e. for very large \(|\vec{r}|\) we have

\[ |\vec{r} - \vec{r}'| = \sqrt{\vec{r}^2 - 2\vec{r}\vec{r}' + \vec{r}'^2} \sim |\vec{r}| - \hat{r}\vec{r}' \]

and therefore

\[ \frac{e^{ik|\vec{r} - \vec{r}'|}}{|\vec{r} - \vec{r}'|} \sim \frac{e^{ik|\vec{r}|}}{|\vec{r}|} e^{-ik\hat{r}\vec{r}'} \]

When applied to \(|\vec{k}\rangle\) this gives

\[
\langle \vec{r} | (H_0 - \frac{k^2}{2} \pm i\epsilon)^{-1} | \vec{k}' \rangle \sim \frac{1}{(2\pi)^3} \int d^3r' e^{-ik\hat{r}\vec{r}'} e^{i\vec{k}' \cdot \vec{r}'} / (2\pi)^3/2 \]

\[
\sim \frac{1}{2\pi \frac{|\vec{r}|}{|\vec{r}'|} (2\pi)^{3/2} \delta(3)(\vec{k} - \vec{k}')}
\]

where \(\vec{k} = k\hat{r}\).

**Note:** Our approximate representation of the integrand only holds for \(|\vec{r}| \gg |\vec{r}'|\). therefore, we will not get an exact \(\delta\)-function for any finite \(\vec{r}\). However, making \(|\vec{r}|\) large enough, we can get as close as we wish to the \(\delta\)-function. That is what we mean by “asymptotic”: go as far with \(\vec{r}\) as needed to approximate a limiting situation within a preset accuracy.

Inserting \(\int d^3k |\vec{k}\rangle\langle \vec{k}|\) into the Lippmann-Schwinger equation we obtain the asymptotic behavior of the scattering solution in the direction \(\vec{r} \parallel \vec{k}\)

\[
\Psi^{(\pm)}_k(\vec{r}) \sim \frac{1}{(2\pi)^{3/2}} \left[ e^{ik\vec{r}} + \frac{e^{\mp ik|\vec{r}|}}{|\vec{r}|} f(\vec{k}', \vec{k}) \right], \quad \vec{k}' = k\hat{r}
\]
4.6 Partial wave scattering solutions

4.6.1 Partial wave expansion

Energy conservation follows from the intertwining property of the Møller operators

\[ SH_0 = \Omega_+^{-1}\Omega_- H_0 = \Omega_+^{-1}H\Omega_- = H_0\Omega_+^{-1}\Omega_- = H_0S. \]

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

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” \( \delta_l(k) \), conventionally written with \( k = \sqrt{E} \):

\[ S|E,l,m\rangle = e^{2i\delta_l(k)}|E,l,m\rangle \]  

(150)

Note that for rotationally symmetric problems there cannot be any dependence on \( m \).

The label \( \alpha \) can be discrete or continuous. Think of polar angles to denote directions, or, alternatively, the corresponding resolution of the rotations in terms of spherical harmonics:

\[ |\alpha\rangle\langle\alpha| = |\phi,\theta\rangle\langle\phi,\theta| = P(\phi,\theta) = \sum_{lm} Y_l^m(\phi,\theta)Y_l^{m*}(\phi',\theta') = \delta(\theta-\theta')\delta(\phi-\phi') \]  

(151)

4.6.2 Spherical Bessel functions

In polar coordinates one can better account for the rotational symmetry and expand plane waves in \( \mathbb{R}^3 \) can be expanded into spherical Bessel functions \( j_l(kr) \) by the formula

\[ e^{ikr} = 4\pi \sum_{l=0}^{\infty} i^l j_l(kr) \sum_{m=-l}^{l} Y_l^m(\hat{k})Y_l^{m*}(\hat{r}). \]  

(152)

The sum over the \( m \)'s can be performed leading to

\[ e^{ikr} = \sum_{l=0}^{\infty} i^l j_l(kr)(2l + 1)P_l(cos\theta). \]  

(153)
Here we denote \( r = |\vec{r}|, k = |\vec{k}|, \hat{k} = \vec{k}/k, \hat{r} = \vec{r}/k \) and \( \cos \theta = \hat{k} \cdot \hat{r} \).

The \( j_l \) obey the radial equation for free motion:

\[
\left[ -\partial_r^2 + \frac{l(l+1)}{r^2} \right] j_l(kr) = k^2 j_l(kr). \tag{154}
\]

For the first few \( l \) we have

\[
\begin{align*}
    j_0(x) &= \frac{\sin(x)}{x} \tag{155} \\
    j_1(x) &= \frac{\sin(x)}{x^2} - \frac{\cos(x)}{x} \tag{156} \\
    j_2(x) &= \left( \frac{3}{x^2} - 1 \right) \frac{\sin(x)}{x} - \frac{3 \cos(x)}{x^2} \tag{157} \\
    \cdots \tag{158}
\end{align*}
\]

They are closely related to the trigonometric functions and, asymptotically at large \( x \), behave as \( \sin(x - l\pi/2)/x \), i.e. they alternate between sin-like and cos-like asymptotic phase.

The \( j_l \) are the regular solutions of this equation that behave as \( \sim r^l \) as \( r \to 0 \), which reflects the “angular momentum barrier”. There is a second type of solutions of Eq. (154) that diverges as \( r^{-l} \) as \( r \to 0 \). The first few of these Neumann functions \( n_l(rk) \) are

\[
\begin{align*}
    n_0(x) &= \frac{\cos(x)}{x} \tag{159} \\
    n_1(x) &= \frac{\cos(x)}{x^2} + \frac{\sin(x)}{x} \tag{160} \\
    n_2(x) &= \left( \frac{3}{x^2} - 1 \right) \frac{\cos(x)}{x} + \frac{3 \sin(x)}{x^2} \tag{161} \\
    \cdots \tag{162}
\end{align*}
\]

The Neumann functions resemble the \( j_l \), but with an additional phase-shift by \( \pi/2 \), which causes the singularity at \( r = 0 \).

The particular linear combinations

\[
h_l^{(\pm)}(x) = n_l(x) \pm i j_l(x) \tag{163}
\]

are called Hankel functions and are convenient for the traditional wave-mechanical investigation of the analyticity of the \( S \)-matrix and scattering
amplitudes. Using these formula, we transform from expressions in $\hat{k}$ and $\hat{k}'$ to expressions in $l$, where the $\delta_l(k)$ appear as the parameters.

**Problem 4.16:** Show that the spherical Bessel-functions are $\delta$-normalized as

$$
\int dr r^2 j_l(kr) j_l(k'r) = \frac{\pi}{2k^2} \delta(k - k')
$$

**Hint:** Use $\langle e^{i\hat{k}\cdot \hat{r}} | e^{i\hat{k}'\cdot \hat{r}} \rangle = (2\pi)^3 \delta(3)(\hat{k} - \hat{k}')$ and compute $\int d\hat{k} Y_l^m(\hat{k}) \langle e^{i\hat{k}\cdot \hat{r}} | e^{i\hat{k}'\cdot \hat{r}} \rangle$ using the plane wave expansion into spherical Bessel functions.

### 4.7 Scattering phases and scattering amplitude

The scattering amplitude in terms of the scattering phases is

$$
f(\vec{k}, \vec{k}') = \sum_l \frac{2l + 1}{k} P_l(\cos \gamma) e^{i\delta_l(k)} \sin \delta_l(k) \tag{164}
$$

where $\cos \gamma = \hat{k}' \cdot \hat{k}$ is the cosine of the angle between $\vec{k}$ and $\vec{k}'$.

**Derivation** First we express the scattering amplitude by the $S$-matrix

$$
S - 1 = -2i\pi \int dE \int \frac{d^3k}{k} \int \frac{d^3k'}{k'}
$$

$$
|\vec{k}\rangle \delta\left(\frac{k^2}{2} - E\right) \langle \vec{k} | V - V(H - E - i\epsilon)^{-1}V | \vec{k}'\rangle \delta\left(\frac{k'^2}{2} - E\right) \langle \vec{k}' |
$$

and

$$
\langle \vec{k} | S - 1 | \vec{k}' \rangle = -2i\pi \langle \vec{k} | V - V(H - E - i\epsilon)^{-1}V | \vec{k}'\rangle \delta\left(\frac{k'^2}{2} - \frac{k^2}{2}\right) \tag{167}
$$

and therefore

$$
\delta(k - k') f(\vec{k}, \vec{k}') = -2\pi ik \langle \vec{k} | S - 1 | \vec{k}' \rangle. \tag{168}
$$

Deriving the final expression for the scattering amplitude is left to the reader in the following problem.

**Problem 4.17:** Starting from the basic expression for the scattering amplitude

$$
\delta(k - k') f(\vec{k}, \vec{k}') = -2\pi ik \langle \vec{k} | S - 1 | \vec{k}' \rangle \tag{169}
$$
derive the scattering amplitude expressed through the scattering phases

\[ f(k, \hat{k} \cdot \hat{k}') = \sum_l \frac{2l + 1}{k} P_l(\hat{k} \cdot \hat{k}') e^{i\delta_l(k)} \sin \delta_l(k) \delta(k - k') \]  

(170)

**Hint:**

1. Substitute the plane wave expansion into spherical harmonics into the equation.
2. Use \( S|k, l, m\rangle = e^{2i\delta_l(k)}|k, l, m\rangle \)
3. Use the \( \delta \)-normalization of the spherical Bessel functions
4. Use \( 4\pi \sum_m Y_{lm}^*(\hat{k}) Y_{lm}(\hat{k}') = (2l + 1) P_l(\cos \gamma) \)

4.7.1 Scattering phases and asymptotic behavior

It is plausible, that at large \( r \), any scattering solution of a spherically symmetric problem for given \( l \) behaves as a linear combination of the regular and irregular spherical Bessel and Neumann functions:

\[ \psi_l^{(\pm)}(r) \sim a_l j_l(kr) + b_l n_l(kr) = c_l \sin(kr + \delta_l(k)) / (kr) \]  

(171)

for some constant \( c_l \). It is easy to show that the phase-shift in the asymptotic behavior is exactly the scattering phase introduced earlier:

**Problem 4.18: Scattering phase and asymptotics** Insert the spherical wave expansion of the scattering amplitude into

\[ \Psi^{(\mp)}(\vec{r}) \sim \frac{1}{(2\pi)^{3/2}} e^{i\delta_l(k)} \left[ e^{\pm ik|\vec{r}|} f(\vec{k}', \vec{k}) \right] , \quad \vec{k}' = k\hat{r} \]  

(172)

and the expansion of the plane wave in spherical Bessel functions to find for \( l \)'th partial wave asymptotic behavior

\[ \langle P_l|\Psi^{(-)}\rangle \sim \sin(kr + \delta_l - l\pi/2) / kr \quad \text{for large } kr \]  

(173)

where \( \langle P_l|\Psi^{(\mp)}\rangle \) means integration over \( \cos \gamma \) only.

**Hint:** Use the orthogonality of the Legendre polynomials \( P_l(\cos \gamma) \) under integration over \( \gamma \) and the asymptotic form of the spherical Bessel functions \( j_l(kr) \sim \sin(kr - l\pi/2) / kr \).
4.8 Analyticity

Analyticity the $T$-matrix is an important property. The starting point is rather simple, namely the fact that the resolvent $R_H(z)$ is analytic (for suitable potentials) in the vicinity of any point $z_0$ where the $R_H(z)$ exists. Consider the resolvent around some $z_0 \in \rho(H)$

$$(H - z)^{-1} = (H - z_0)^{-1}[1 + (z - z_0)(H - z)^{-1}]$$ \hspace{1cm} (174)

$$= (H - z_0)^{-1}\sum_{n=0}^{\infty}[(z - z_0)(H - z_0)^{-1}]^n.$$ \hspace{1cm} (175)

Where it converges, the series is analytic in $z$. From the spectral representation of $H$ it is easy to see that $||(H - z_0)^{-1}|| \leq |\Im z_0|$. Therefore, the series is norm-convergent for all $|z - z_0| < |\Im z_0|$ and, as bounded operators form a Banach space, defines a family of operators that depends analytically on $z$.

4.9 Analytic functions

The fact that an analytic function has — at least locally — a convergent series expansion, has far reaching consequences. A brief reminder:

- A function is analytic in a region $M$, if and only if it is differentiable (as a complex function) at every point.

- Integration along a closed (simply connected) path gives 0 (Cauchy theorem)

- Integration by residue theorem, in case of poles.

- An analytic function is infinitely many times differentiable.

- Any two analytic functions on two distinct, but overlapping regions. If they coincide on a line segment in the overlapping region, they are identical on the analyticity region that they share. Either is the unique analytic continuation of the other.

- **Caution:** complex conjugation is not an analytic map, $f(z)$ analytic does not imply that $f(z)^*$ is analytic, but $g(z) = [f(z^*)]^*$ is analytic.
• A simple consequence: if \( f(z) \) is analytic on a region \( R \) that includes a segment of the real axis, then \( f(z^*)^* = f(z) \) on \( R \cap R^* \) and the two functions are the unique analytic continuation of each other.

Analytic functions are rather robust under summation and integration:

\[
f(z) = \sum_{n=0}^{\infty} f^{(n)}(z)
\]

is analytic, if each \( f^{(n)} \) is analytic and convergence is uniform.

Let \( g(z,r) \) be a function that is analytic w.r.t. \( z \) in some region \( R \) and continuous w.r.t. \( r \) on \( r \in [a,b] \). Then

\[
f(z) = \int_{a}^{b} drg(z,r)
\]

is analytic. If we can establish uniform convergence on \([a,b]\), the function may be singular at the end points and the integral can extend to \( \infty \).

4.10 Analyticity of \( S(k) \)

Analyticity is better discussed for the modulus w.r.t. momentum \( k := \sqrt{2E} \), rather than energy \( E \). By the fact that \( \Omega_+ \neq \Omega_- \), we know that the analytic \( \Omega(E) \) is discontinuous at \( E \in \mathbb{R}_+ \), i.e. the positiv half-axis is a “branch cut” of \( \Omega(E) \). When considered as a function of \( k \) instead, the branch cut is unfolded into the whole real axis: the point where the discontinuity in \( E \) had occured are separated into the positive and negative sides of the real axis. In that way the \( \lim_{\epsilon \downarrow 0} \), converts to a limit from the upper complex \( k \)-plane towards the real axis, the \( \pm \) signs corresponding to limits to the positive and negative part of the real axis, respectively. Spectral values \( E < 0 \) are mapped into \( k = i\sqrt{(2|E|)} \), i.e. points on the positive imaginary \( k \)-axis. Except for these, we can hope for analyticity in the whole upper half plane.

Rigorously, analyticity in the upper half plane can be proven for a mildly restricted class of potentials: one needs that the operator \( V^{1/2}(H_0 - k^2/2 - i\epsilon)^{-1}|V^{1/2}| \) is a “Hilbert-Schmidt” operator. That condition is somewhat stronger than “compactness” of \( V(H_0 - k^2/2 - i\epsilon)^{-1} \). For negative \( V \), the square root are to be understood as \( V(r)^{1/2} := \text{sign}(V(r))|V(r)|^{1/2} \).
The fact that the discontinuity at the branch cut disappears opens the chance to analytically continue $\Omega(k)$ into the lower half of the complex $k$-plane. In terms of energy, we slip onto the “second Riemann sheet”. However, the possibility to actually analytically continue has only been proven for a rather restricted class of short range potentials that fall off as the Yukawa potential. The fact that scattering theory exists (i.e. the Møller operators exist and are asymptotically complete) does by no means guarantee that analytic continuation is possible.

If we can continue it into the lower half plane, poles in $\Omega(k)$ (and with it poles in $T$) can (and often will) occur. These are on the second Riemann sheet of energy: if we were able to rotate the branch cut, we might uncover those energy-poles. Indeed, there is such a procedure, named “complex scaling” of the Hamiltonian.

We can now write the Møller operators as

$$\Omega_{\pm} = \int d\phi d\eta \int dk k \Omega(i\epsilon \pm k)\delta(H - k^2/2). \quad (178)$$

with, for complex $k$,

$$\Omega(k) = 1 - (H - k^2/2)^{-1}V = [1 + (H_0 - k^2/2)^{-1}V]^{-1} \quad (179)$$

Similarly we write representation of the $T$-operator w.r.t. $k$ as

$$t(k) = V\Omega_-(k) = V - V(H - k^2/2)^{-1}V. \quad (180)$$

This is an analytic function of $k$ in the upper complex plane.

**Problem 4.19:** S how the above form of the $S$-matrix by formal algebraic manipulations of $t(k)$

(a) (assume, for simplicity, that $V > 0$)

$$t(k) = [V^{-1} + (H_0 + k^2)^{-1}]^{-1} = t^\dagger(-k^*)$$

(b)

$$t^{-1}(k) - t^{-1}(-k) = 2\pi i \delta(H_0 - k^2/2)$$

(c)
With that the **spectral representation of the S-matrix** can be written as

\[ S = \int_{0}^{\infty} dkkS(k)\delta(H - k^2/2) \]  
\[ S(k) = t^{-1}(-k)t(k) \]  
\[ = s- \lim_{\epsilon \downarrow 0} [1 + (H_0 - k^2/2 + i\epsilon)^{-1}V][1 + (H_0 - k^2/2 - i\epsilon)^{-1}V]^{-1} \]  

\[ (181) \]
\[ (182) \]
\[ (183) \]

### 4.10.1 Rapidly decaying potentials

Analyticity properties have been proven for potentials that fall off rapidly. A typical example is the Yukawa potential

\[ V(r) = V_0 \frac{e^{-\mu r}}{r}, \quad \mu > 0. \]  

\[ (184) \]

A slightly more technical (and more general) criterion is that the integral

\[ \|V^{1/2}(H_0 - k^2/2)^{-1}V^{1/2}\|^2 = \int d^{(3)}r d^{(3)}r' \frac{V(\vec{r})V(\vec{r}')}{(4\pi|\vec{r} - \vec{r}'|)^2} e^{i(k-k')|\vec{r} - \vec{r}'|} \]  

\[ (185) \]

remains finite for also for negative imaginary parts of \( k \), i.e. when the exponential in the integrand would be growing.

### 4.10.2 Poles of \( S \)

In traditional representations of scattering theory, the analytic structure is usually discussed in terms of the “Jost functions”. This is equivalent to studying \( S(k) \) in the form (183). To connect to the traditional discussion (not given here), one defines yet another quantity

\[ D(k) = 1 + V^{1/2}(H_0 - k^2/2)^{-1}|V|^{1/2} = V^{1/2}t^{-1}(k)|V|^{1/2} \]  

\[ (186) \]

(we mean \( V^{1/2} := \text{sign}(V)|V|^{1/2} \)) and re-write (183)

\[ S(k) = V^{-1/2}D(-k)^{-1}D^{-1}(k)|V|^{1/2} \]  

\[ (187) \]

Here we assume that the potential is such that the analytic continuation can be done into the lower complex half \( k \)-plane down to some \( \Re m \vec{k} \geq \kappa_0 < 0 \). Poles in \( S(k) \) will appear, where \( D(k) \) has a zero or \( D(-k) \) has a pole.
The rapidly decaying condition implies that \( V^{1/2}(H_0 - k^2/2)^{-1}|V|^{1/2} \) has at most a finite number of eigenvalues = \(-1\) (for given \(k\)). In the upper half plane there are no poles of \(D(k)\) (by the analyticity of the resolvent). There are only zeros at strictly imaginary \(k\) for the bound state energies \(E_n = k^2/2, E_n < 0\).

As \(D(k)\) and \(D(k^\star)\) are related by time-reversal \((i \rightarrow -i)\) and \(D(k) = D^\dagger(k^\star)\) (as shown for the \(t(k)\)), \(D(k)\) and \(D(-k)\) assume there poles at the same \(k\) (when and operator is zero, obviously also its adjoint is zero, same for divergence). This ensures that \(S(k)\) remains non-zero and non-singular, where it is analytic.

The zeros of \(D(k)\) and \(D(-k)\) correspond to

\[
0 = D(k)\psi = \psi + V^{1/2}(H_0 - E)^{-1}V^{1/2}\psi
\]  

(188)

Writing \(\phi = (H_0 - E)^{-1}V^{1/2}\psi\) we are lead back to the Schrödinger equation \((H_0 + V - E)\phi = 0\). For the kind of short range potentials that we consider here, the bound states of this appear only at negative \(E\). We have not developed the instruments to show this here, it is related to a theorem that relatively compact potentials generate at most a finite number of bound states at negative energies. In terms of classical physics, such potentials generate an only finite phase space volume below \(E = 0\).

A priori, \(D(k)\) is not defined in the lower half plane, but it may be analytically continued to there. Upon analytical continuation we may encounter zeros of \(D(k)\) in the lower half complex plane at \(\Re(k) \neq 0\). These will cause structures in the scattering amplitudes that correspond to resonances. Finally, upon analytic continuation, also poles of \(D(k)\) may appear. These are not usually associated with physical meaning.

4.11 Levinson theorem

The fact that the poles in the upper half plane all correspond to bound states indicates that we should be able to count the bound states by integrating around them in with an infinite half-circle in the upper half plane. For the integral at the infinite half-circle not to contribute we need, as always, some technical constraints that ensure that the integrand drops faster than \(|z|^{-1}\) for large \(|z|\).
**Theorem 5.** (Levinson) Let $N_b$ the number of bound states then

$$2\pi N_b = i \lim_{k \to \infty} \det(S(k)) = i \lim_{k \to \infty} \text{Tr} \log(S(k))$$

(189)

under the condition that $V$ is relative compact to $H_0$ and $\text{Tr}(\mathbb{I}(H_0 - z)^{-1} - (H-z)^{-1}) < M(z)$ where $M(z) \subset \mathcal{O}(|z|^{-1-\epsilon})$ for $|z| \to \infty$ and $\mathcal{O}(|\Re m z|^{-1+\epsilon})$ and $\log S(0) = 0$ (requires that there is no bound state of $H$ at 0.)

4.11.1 Ingredients of the proof

Remember the Riesz projectors:

$$\frac{1}{2\pi i} \int_{C_b} dz (H - z)^{-1} = \sum_{E_b} \sum_{\alpha} |E_b, \alpha \rangle \langle E_b, \alpha|,$$

(190)

where $E_b$ are the bound states inclosed by the integration path $C_b$. The trace of that is the number of bound states, counting also possible multiplicities (here labelled by $\alpha$).

The condition on the trace of the difference is not very strong and a standard part of the proof asymptotic completeness. Here it is used for ensuring that the following formal manipulations correct. We write

$$Q_{\pm} = 1 + (H_0 - E \pm i\epsilon)^{-1}V, \quad S(E) = Q_+(E)Q_-^{-1}(E).$$

(191)

We may then calculate inside the Tr just as with ordinary functions (paying attention to not permuting operators) VERIFY

$$\text{Tr} \frac{d}{dE} \log S(E) = \text{Tr} Q_- Q_+^{-1} [Q_+^1 Q_-^1 - Q_+ Q_-^{-1} Q_+^1 Q_-^{-1}]$$

$$= \text{Tr}(Q_+^{-1}Q_+' - Q_-^{-1}Q_-')$$

$$= \text{Tr} \left[ 1 + (H_0 - E \pm i\epsilon)^{-1}V \right]^{-1} (H_0 - E + i\epsilon)^{-2}V - (\epsilon \leftrightarrow -\epsilon)$$

$$= \text{Tr} \left[ (H_0 - E + i\epsilon)^{-1} - (H - E - i\epsilon)^{-1} - (\epsilon \leftrightarrow -\epsilon) \right]$$

Now we can integrate over $E$, which we can write as an integral around the real axis:

$$\text{Tr} \log S(E) = \text{Tr} \int_C dz \left[ (H - z)^{-1} - (H_0 - z)^{-1} \right]$$

(192)

(see path). By assumption about $M(z)$, closing the large circle does not give a contribution, and neither does $(H_0 - z)^{-1}$ as $\sigma(H_0)$ is completely outside the path. Refer to the Riesz projectors for completing the proof.
4.11.2 Spherically symmetric case

The somewhat scary “trace of a log of an operator” becomes rather transparent in the case of rotational symmetry: for given partial wave, $S_l(E)$ is a function of $E$ and acts as multiplication in a 1-d space:

$$S_l(E) = \exp[2i\delta_l(E)], \quad \text{Tr}[\log S_l(E)] = 2i\delta_l(E) : \quad (193)$$

the integral of the phase-shift over energies from 0 to $\infty$ tells us about the number of the system’s bound states!.

In the more general case, the meaning of $\text{Tr} \log S$ is readily seen in the spectral representation.

4.12 The delay operator

One can illustrate a typical resonances as a quasi-bound state, that traps a scattering particle momentarily and releases it later. Apart form general handwaving arguments about associating a line-width $\Gamma$ with a life-time $\tau = 2\pi/\Gamma$, so far no relation between peaks of the scattering cross section and any time has been established. To do that, one first defines a “delay operator” and then shows how it relates to cross-sections, in the simplest case through phase-shifts $\delta_l(E)$.

Let $\chi_R$ the characerisitc function of a sphere with radius $R$. Then

$$\int_{-\infty}^{\infty} dt \langle U_t \psi | \chi_R | U_t \psi \rangle = \langle \psi | \int_{-\infty}^{\infty} dt \tau_t(\chi_R) | \psi \rangle$$ \hspace{1cm} (194)

is the time that a given wave-packet $\psi$ spends in the sphere. Note that, if $\psi$ has any bound state content, the integral will diverge. Here we have defined the time-evolution of an operator $A$ (Heisenberg picture) as $\tau_t(A) = \exp(itH)A \exp(-itH)$, similarly $\tau_t^0(A)$ for $H_0$.

A delay can now be defined as the difference in time spent in a sphere under free motion $\tau_0$ and scattering motion $\tau$. In order to compare equivalent wave packets, we choose the free wave packet as $\phi$ and the scattering wave packet as $\psi = \Omega_- \phi$, i.e., in the far past they agree. By the intertwining property of the Møller operators we find

$$\langle \psi | \tau_t(\chi_R) | \psi \rangle = \langle \phi | \Omega_-^\dagger \tau_t(\chi_R) \Omega_- | \phi \rangle = \langle \phi | \tau_t^0(\Omega_-^\dagger \chi_R \Omega_-) | \phi \rangle$$ \hspace{1cm} (195)
and we can compare, for any $\phi \in \mathcal{H}$ the delays at given $R$:

$$
\langle \phi | D_R | \phi \rangle = \langle \phi \mid \int_{-\infty}^{\infty} dt \tau_t^0 (\Omega_-^\dagger \chi_R \Omega_- - \chi_R) | \phi \rangle .
$$

(196)

In order to eliminate the arbitrary choice of $R$ we take $R \to \infty$. For seeing that this makes sense, consider the case that $H_0$ and $H$ agree exactly on $R > R_0$: then the limit is reached already at $R_0$. If this is not the case (and still the limit exists, alas not for Coulomb!) one captures any miniscule delay caused by some increasingly tiny potential and one obtains the

**Delay operator**

$$
D := w - \lim_{R \to \infty} D_R = -iS^{-1} \int_0^\infty dE \delta(H_0 - E) \frac{dS(E)}{dE}.
$$

(197)

The second equation needs to be shown. Before that, we remark that again there appears something like the derivative of the log of $S$, which we can identify with the phase-shift $\delta_l(E)$ in the simple case of spherical symmetry.

4.12.1 Derivation of the delay operator

As usual here, we give a rather formal derivation, which however should show what happens.

- We first reexpress $D_R$ using $S$. For that one uses the fact that, the operator from infinitely large negative times to 0

$$
\int_{-\infty}^0 dt \tau_t^0 (\Omega_-^\dagger \chi_R \Omega_- - \chi_R) \xrightarrow{w} 0
$$

(198)

Bypassing all important questions about whether we can interchange the $\lim_{R \to \infty}$ with integration, this becomes a triviality. $\lim_{R \to \infty} \chi_R = 1$ and $\Omega \pm^\dagger \Omega \pm = 1$.

- For the integration $[0, \infty)$ we use $\Omega_- = \Omega_+ \Omega_+^\dagger \Omega_- = \Omega_+ S$ and the fact that $S$ is invariant under free time-evolution $\tau_t^0(S) = S$. With that one
obtains
\[ \int_0^\infty dt \tau^0_t (\Omega^\dagger \chi R \Omega - \chi R) = \int_0^\infty dt \tau^0_t (S^{-1} \chi R S - \chi R) \]
\[ + S^{-1} \int_0^\infty dt \tau^0_t (\Omega^\dagger \chi R \Omega + - \chi R) \]

For the further steps, one switches back into a time-dependent picture for the \( S \):
\[ S = \int dt' \tilde{S}(t') e^{it'H_0} \]  
(199)
where \([\tilde{S}(t), H_0] = 0\)

One writes \( D_R = S^{-1} \int_0^\infty \int_0^\infty \tilde{S}(t') e^{it'H} \) which after some manipulation reduces to
\[ S^{-1} \int_0^\infty \int_0^\infty dt' \tilde{S}(t') e^{it'H_0} = -i S^{-1} \int_0^\infty \delta(H_0 - E) \frac{dS(E)}{dE}. \]  
(200)

4.12.2 Resonances

If there is a resonance in the sense that \( D(k) \) has a zero at \( k = k_r - ib \) in the lower half plane, near the real axis, we can write
\[ S(k) = V^{-1/2} D(-k)^{-1} D^{-1}(k) |V|^{1/2} = \frac{(-k - k_r + ib)(-k + k_r + ib)}{(k - k_r + ib)(k + k_r + ib)} \times g(k), \]  
(201)
where \( g(k) \) is some function that varies slowly near \( k_r \). Then
\[ -i \frac{d}{dk^2/2} \log(S(k)) \approx \frac{b}{k} \left[ \frac{1}{(k - k_r)^2 + b^2} + \frac{1}{(k + k_r)^2 + b^2} \right] \]  
(202)
For small \( b \ll k_r \), this has a \( \delta \)-like peak which makes a large, the dominant contribution to the delay, if we choose our wave-packet \( \phi \) to be concentrated near \( E_r = k_r^2/2 \).
4.13 Properties of the scattering amplitude

“On shell”, i.e. for real $k$, we have

$$f(k; \hat{k}, \hat{k}') \neq f^*(k; \hat{k}', \hat{k}) = \frac{ik}{2\pi} \int d\hat{k}'' f(k, \hat{k}, \hat{k}'') f(k, \hat{k}', \hat{k}'')$$  \hspace{1cm} (203)

$$f(k, \hat{k}', \hat{k}) = f(k, -\hat{k}, -\hat{k}')$$ for time-reversible systems  \hspace{1cm} (204)

$$f(k, \hat{k}', \hat{k}) = f(k, -\hat{k}', -\hat{k})$$ for reflection invariant systems  \hspace{1cm} (205)

The first identity results from the **Low equation** for the $t(k)$:

$$t(-k) - t(k) = 2\pi it(k)\delta(H_0 - k^2/2)t(-k).$$  \hspace{1cm} (206)

which can be (formally) obtained from

$$t(k)[t^{-1}(k) - t^{-1}(-k)]t(-k) = t(k)[2\pi i\delta(H_0 - k^2/2)]t(-k).$$

4.13.1 Optical theorem

For $\hat{k} = \hat{k}'$ the rhs. integral in (203) is essentially the total cross section

$$\sigma_t(k) = \frac{4\pi}{k} \Im f(k, \hat{k}, \hat{k}) : \hspace{1cm} (207)$$

the imaginary part of the forward scattering amplitude reflects the total cross section. (Sounds plausible, if we associate with the imaginary part amplitudes that actually do not continue in that direction). Note that this holds for general potential scattering, not just spherically symmetric problems.

4.13.2 Reciprocity

Time reversal of the original problem guarantees that we can go back the way we came. Of course, we must interchange the roles of incoming and outgoing angles $\hat{k} \leftrightarrow \hat{k}'$ and revert the directions.

4.13.3 Detailed balance

In many simple statistical arguments one uses an assumption about “detailed balance”, the fact that the cross section for going from $\hat{k} \rightarrow \hat{k}'$ equals the cross section for the reverse process:

$$\sigma(k, \hat{k}, \hat{k}') = \sigma(k, \hat{k}', \hat{k}).$$ \hspace{1cm} (208)
Note that this is more than reciprocity (time-reversal), as it also requires reflection symmetry. This becomes quite obvious if one considers scattering from targets that are not reflection symmetric.

### 4.13.4 Unitarity limit

In spherical symmetry we get from (164)

\[
\sigma_t = \sum \sigma_l, \quad \sigma_l(k) = \frac{4\pi}{k^2} (2l + 1) \sin^2 \delta_l(k).
\]  \hspace{1cm} (209)

We see that the partial wave cross sections are bounded by the “unitarity limit”

\[
\sigma_l \leq \frac{4\pi}{k^2} (2l + 1).
\]  \hspace{1cm} (210)

The name refers to the fact that the general form of the partial wave amplitude is an immediate consequence of the unitarity of \( S \).

Assume purely resonant scattering, i.e.

\[
S_l(k) = e^{2i\delta_l(k)} = \frac{k - k_r + ic}{k - k_r - ic}
\]  \hspace{1cm} (211)

then \((\Re(e^{i\delta_l})^2 = 1 - 2 \sin^2 \delta_l)\)

\[
\sigma_l = \frac{4\pi}{k^2} (2l + 1) \frac{c^2}{(k - k_r)^2 + c^2}.
\]  \hspace{1cm} (212)

It is interesting to note that that limit is just 4 times the surface of an annulus for the classical impact parameters \( kb_l = l\hbar \) and \( b_{l+1} \) as its lower and upper radii

\[
\frac{4\pi}{k^2} = 4\pi (b_{l+1}^2 - b_l^2)
\]  \hspace{1cm} (213)

### 4.13.5 Scattering length

The unitarity limit does not impose any constraint on the behavior for \( k \to 0 \). Yet, for most standard potentials one can show that \( \delta_l(k) \sim k^{2l+1} \) for \( k \to 0 \).

This can be thought of as a result of the “centrifugal barrier” and can be made plausible by looking at the first Born approximation of the \( l \)th
partial wave of a potential with finite range \( V(r) = 0 \) for \( r > R \):

\[
f^{(1)}_l \propto \int_0^R dr r^2 j^2_l(kr)V(r) \int d\Omega |Y^m_l(\Omega)|^2 \tag{214}
\]

\[
= \int_0^R dr r^2 j^2_l(kr)V(r) \tag{215}
\]

\[
\approx \frac{(4\pi)^2}{(2l+1)!} \int_0^R dr r^2(kr)^{2l+1}V(r) \tag{216}
\]

\[
\propto k^{2l} \int_0^R dr r^{2l+2}V(r). \tag{217}
\]

Here we have used the behaviour \( \sim (kr)^l \) of the \( j_l(kr) \) for small \( kr \): The partial wave contributions go to zero like \( k^{2l} \). The \( s \)-wave scattering amplitude \( (l = 0) \) approaches a constant, looking at (164) we see that indeed \( \delta_0(k) \sim k \) at small \( k \).

We define the **scattering length**

\[
a = -\lim_{k \to 0} \frac{\delta_0(k)}{k} = -f(0, \hat{k}, \hat{k}). \tag{218}
\]

The sign is chosen such that the positive sign is for repulsive potentials, again referring to the first Born approximation (which, btw. is totally unjustified, although not necessarily totally wrong for low energy scattering):

\[
\text{sign}(a) = -\text{sign}(f(k = 0)) \approx -\text{sign}(f^{(1)}(k = 0)) = \text{sign}(\langle \vec{k} | V | \vec{k} \rangle) \tag{219}
\]

Low energy scattering is usually only “\( s \)-wave scattering”, i.e. scattering with \( l = 0 \), in traditional terminology the \( s \)-wave:

\[
\sigma_{tot}(k \to 0) \approx \sigma_0(k \to 0) = 4\pi a^2 \tag{220}
\]

4.14 Computational techniques

4.14.1 The Born series

The Lippmann-Schwinger equation (98) is an integral equation that will also be difficult to solve directly. However, one can iterate it (signs are
easier, when we write \(- (H_0 - E \pm i\epsilon)^{-1} = (E - H_0 \mp i\epsilon)^{-1}\)

\[ |\Psi^{(\mp)}\rangle = |\vec{k}\rangle \]

\[ + (k^2/2 - H_0 \pm i\epsilon)^{-1} V|\vec{k}\rangle \]

\[ + (k^2/2 - H_0 \pm i\epsilon)^{-1} V(k^2/2 - H_0 \pm i\epsilon)^{-1} V|\vec{k}\rangle \]

\[ + (k^2/2 - H_0 \pm i\epsilon)^{-1} V(k^2/2 - H_0 \pm i\epsilon)^{-1} V(k^2/2 - H_0 \pm i\epsilon)^{-1} V|\vec{k}\rangle \]

etc. . .

If \(V\) is “small” in some sense compared to \(k^2/2 - H_0 \pm i\epsilon\) one can terminate the series at finite iterations. Unfortunately, \(E = k^2/2\) is in the continuous spectrum of \(H_0\), i.e. there are vectors on which \(E - H_0\) is arbitrarily small and \((E - H_0 \pm i\epsilon)\) would become very large \(\sim 1/\epsilon\). We are only safe if these vectors do not appear in \(V|\vec{k}\rangle\). This is case-dependent. Convergence or useful approximation properties of the Born series are not guaranteed and, in fact, very often not given in practice.

In spite of these doubts, we can write the scattering amplitude (say, post form)

\[-\frac{1}{2\pi^2} f(k, \hat{k}, \hat{k}^\prime) = \langle \vec{k}|V|\Psi^{(-)}_{\hat{k}_0}\rangle \]

\[ = \langle \vec{k}|V|\vec{k}'\rangle + \langle \vec{k}|V(k^2/2 - H_0 + i\epsilon)^{-1} V|\vec{k}'\rangle \]

\[ + \langle \vec{k}|V(k^2/2 - H_0 + i\epsilon)^{-1} V(k^2/2 - H_0 + i\epsilon)^{-1} V|\vec{k}'\rangle + \ldots \]

We have used the first term of this series as the “first Born approximation” \(f^{(1)}\) of the scattering amplitude. In real life, one rarely goes beyond the term second order in \(V\), i.e. \(f^{(2)}\).

The popularity of the Born approximation is due to its feasibility and the lack of alternatives. Even before the feasibility of the computation there should be the question of convergence. On the other hand, there are well-known cases, where a series does not converge, but still the first few terms can give useful information (such is the case in some perturbation series).
4.14.2 Kohn variational principle

We may try to guess an approximate potential \( V_g \approx V \) for which, one way or another, we can compute the resolvent and wave operators \( \Omega_g(k) \) for \( H_g = H_0 + V_g = H + (V_g - V) \), and the corresponding \( T_g(k) \).

**Problem 4.20: Kohn variational principle** Derive

\[
T(k) = T_g(k) + \Omega^\dagger_g(k)(V-V_g)\Omega_g(k) - \Omega^\dagger_g(k)(V-V_g)(H-k^2/2)^{-1}(V-V_g)\Omega_g(k)
\]

We get identity for the \( T \)-matrices, the Kohn variational principle

\[
T(k) = T_g(k) + \Omega^\dagger_g(k)(V-V_g)\Omega_g(k) - \Omega^\dagger_g(k)(V-V_g)(H-k^2/2)^{-1}(V-V_g)\Omega_g(k)
\]

The last term is quadratic in \( V-V_g \), so if this is small we may obtain a good approximation by only the computable first two terms.

In some cases this allows analytical estimates. More importantly, it allows for systematic improvement of the result in a numerical approach.

4.15 Standard textbook examples

4.15.1 Hard sphere scattering

**Problem 4.21: Hard sphere** A hard sphere is described by the potential

\[
V(\vec{x}) = \begin{cases} 
+\infty & r < R \\
0 & r \geq R 
\end{cases}
\]

Evaluate the \( s \)-wave scattering amplitude for this system.

**Problem 4.22:** Give the hard sphere scattering phase \( \delta_l(k) \) for \( l = 1 \). What is the behavior for small \( k \) ?

The total cross section at low energies can be calculated by observing that (1) only \( s \)-wave scattering contributes and (2) the \( s \)-wave amplitude does not depend on the scattering angle:

\[
\sigma_{tot} \approx \int d\Omega \frac{d\sigma_0}{d\Omega} = 4\pi \frac{\sin^2(-kR)}{k^2} \approx 4\pi R^2 \quad \text{for small } k
\]

Note: the total cross section is 4 times the geometrical cross section \( R^2\pi \).
Quantum scattering is more than just casting shadows. At the least, it also accounts for the fact that those parts that are missing in the forward direction show up in some other direction — which would account for a factor of 2, which is true in the high-energy limit.

4.15.2 Spherical potential scattering: Ramsauer-Townsend effect

We now replace the infinite repulsive potential of the hard sphere by an attractive (negative) finite potential and restrict our considerations to the $s$ wave again.

We have already seen that low-energy scattering is usually dominated by the $s$-wave ($l=0$). In that case the three-dimensional scattering problem is effectively reduced to a 1-dimensional one.

**Problem 4.23: Ramsauer-Townsend effect** Use the spherical well potential

$$V(\bar{x}) = \begin{cases} V_0 < 0 & \text{for} |\bar{x}| < R \\ 0 & \text{else} \end{cases} \quad (231)$$

(a) Set up the equations for matching values and derivatives at $R$.

**Hint:** The problem can be reduced to scattering from a finite potential well in one dimension, which is found in literature.

(b) Starting from $V_0 = 0$, lower the potential such that $\sqrt{k^2 - 2V_0R}$ will pass through $(2n+1)\pi/2$. Conclude that there is a resonance near by.

(c) Argue that the phase shift goes through 0 at low energies and the cross section passes through 0 at some point (Ramsauer-Townsend effect).

**Hint:** At low energies, approximate the trigonometric functions by their Taylor series.

**Resonant scattering:** One interesting case arises when we lower $V_0$ such that $qR = \sqrt{k^2 - 2V_0R}$ passes the a value $(2n+1)\pi/2$: at these points the inner part of the wave function $\sin qx$ has an anti-node at $R$. If $kR$ is not too large, i.e. in low energy scattering, $\delta_0$ also passes through $\pi/2$ near these points. The cross section

$$\sigma_0 = \frac{4\pi}{k^2} \sin \delta_0(k) = \frac{4\pi}{k^2} \quad (232)$$
reaches the unitarity limit. This is in essence what is a resonance in scattering: there is an energy match of the inner range with the scattering energy.

**Ramsauer-Townsend effect:** Another interesting case arises for values of $V_0$ where $\alpha - kR = (2n + 1)\pi$. Using the Taylor expansion of $\arctan$ we see that such points are reached

The scattering phase goes through $\delta_0(k) = 0$ and also the $s$-wave cross section has a 0 at this point. If energies are low enough

$$\sigma_{\text{tot}} \approx \sigma_0 = \frac{4\pi}{k^2} \sin \delta_0 = 0!$$ (233)

the object becomes transparent!

Historically this is an important effect: such behavior was indeed observed in electron scattering from noble gas atoms. At the time of its first observation, there was no way of explaining the decrease of the cross-section with increasing energy to the “Ramsauer-Townsend minimum”. We see why: it is a distinctly wave-mechanical effect as the wave-length $qR$ must just match the “length” of the potential.

![Fig. 9.6 Ramsauer effect. Minimum in cross section for scattering of electrons by xenon at about 1 eV. (After S. G. Kukolich, Am. J. Phys. 36, 701 (1968).)](image)

**Problem 4.24:** Write down the solutions for spherical well $s$-wave scattering for values of $V_0$ such that $qR = n\pi$ and $qR = (2n + 1)\pi/2$, assuming small $k$. What is the ratio of the amplitudes of the $s$-wave function $r\Psi(r)$ inside and outside the potential radius $R$? For which of the two values do we get higher amplitude in the range $r < R$? Discuss the meaning of this and
make a drawing of the solutions for some (small) $k$.

**Problem 4.25:** Draw the functions $kR$, $kR - \pi$ and $\alpha(k)$ and show graphically the conditions $\delta_0 = \pi$ and $\delta_0 = \pi/2$. Use the Taylor expansions of $\arctan x = x - x^3/3 + \ldots$ and $1/\arctan = x + x^3/3 - \ldots$ to determine more precisely the locations in $k$ of the resonance $\delta_0 = \pi/2$ with lowest $k$ and of the Ramsauer-Townsend minimum $\delta_0 = \pi$ in low energy scattering.

## 5 Complex scaling

We have seen that the resolvent $R_z(H) = (H - z)^{-1}$ plays a central role for scattering. While from our discussion we have no direct proof of the connection between poles of the $S$-matrix and the analytic structure of $R_z(H)$, we may expect that the analytic structure of $H$ is related to that of $S$. Note that we have analytically continued $S(k)$. We can also — in suitable cases — analytically continue the Hamiltonian itself. This starts from the observation that we can define a unitary scaling transformation on $L^2(\mathbb{R}^d, d^n(x))$ by

$$U_\lambda : (U_\lambda \Psi)(x) = e^{n\lambda/2} \Psi(e^{n\lambda}x), \lambda \in \mathbb{R}. \quad (234)$$

This amounts to changing the units of length and, as a unitary transformation, does not change any of the “physics” associated with the Hamiltonian. The time-dependent Schrödinger equation transforms as

$$i \frac{d}{dt} \Psi(x) = H \Psi(x) \rightarrow i \frac{d}{dt} \Psi_\lambda(x) = H_\lambda \Psi_\lambda(x), \quad \Psi_\lambda := U_\lambda \Psi_0, \quad H_\lambda := U_\lambda H U_\lambda a^\dagger. \quad (235)$$

Importantly, the $\sigma(H_\lambda) = \sigma(H)$, as the spectrum is invariant under unitary transformation. The actual shape of $H_\lambda$ and of $\Psi_\lambda$ do depend on $\lambda$. For example, for the Hydrogen atom

$$H_\lambda = -\frac{1}{2} e^{-2\lambda} \Delta - e^{-\lambda} \frac{1}{r}. \quad (236)$$

This transformation can be exploited to analytically continue the Hamiltonian to non-selfadjoint values. Naively, we consider $H_\lambda$ as an operator-valued function for $\lambda$ on the real axis. In some cases, such as the Hydrogen
atom, the formal continuation into the complex plane is simple (the factor $i$ in $i\theta$ is traditionally kept separate):

$$H_\theta = -\frac{1}{2} e^{-(i\theta) \Delta} - e^{i\theta} \frac{1}{r}, \quad \theta \in \mathbb{C}. \quad (237)$$

We postpone the discussion of the meaning of “analyticity” for an unbounded operator and of the domain of the transformed $D(H_\theta)$, first consider the spectrum. Instead, we naively discuss the spectrum, first the bound states. For the real scaling $\mathbb{R} \ni \lambda = -i\theta$ we know that the bound state energies remain unchanged

$$E_n(\lambda) \equiv E_n(0). \quad (238)$$

Assuming analyticity (to be discussed), we see that also for complex $\theta$ the bound state spectrum remains unchanged:

$$E_n(\theta) \equiv E_n(0) \quad \text{for bound state energies.} \quad (239)$$

What about the continuous spectrum? It does not remain unchanged. The reasoning about an isolated energy that would be constant is not applicable: although the continuous spectrum as a whole does not change, the $\sigma_{ac}(H) = [0, \infty)$ can be considered as being stretched (or shrunk) by scaling. E.g., for free motion $H = -\Delta$, we may consider the non-Hilbert eigenfunctions $e^{ikx}$, and we immediately see that the eigenvalue going with this moves under scaling. We know that $\sigma(-\Delta) = [0, \infty)$ and we immediatley see that

$$\sigma(-e^{2i\theta} \Delta) = e^{-2i\theta}[0, \infty) = e^{-2i\Re(\theta)}[0, \infty) : \quad (240)$$

the spectrum rotates into the complex plane by the angle $-2\theta$. Interestingly, the exact same happens for generaly, suitably analytic $H_\theta$: the continuous spectrum rotates into the complex plane by $-2\Re(\theta)$.

The explanation for the general case uses a theorem similar to the one that we had envoked justify that a relatively compact potential at most adds a finite number of bound states to $-\Delta$, but leaves the continuous spectrum invariant. This theorem is, in fact, not limited to self-adjoint operators, it requires only that $H_0$ and $V$ are relativ compact: let $z \notin \sigma(H_0) \cup \sigma(H_{0,\theta} = e^{-2i\theta} H_0)$. Then, if $(H_0 - z)^{-1} V$ is compact, also

$$(H_{0,\theta} - z)^{-1} V = e^{2i\theta}(H_0 - e^{2i\theta}z)^{-1} V$$
is compact (this follows from the analyticity in $z$). So, adding a (relatively compact) potential does not change the continuous spectrum of $H_0 = -e^{-2i\theta}[0, \infty)$.

5.0.1 Resonances

The interesting twist is that the extra “bound states” (i.e. point spectrum) can now appear anywhere in the complex plane, as the operator is not self-adjoint. We already know that the bound states will appear where they had been. In addition, it turns out that in the wedge between the positive real axis and the continuous spectrum, point spectrum can appear at complex values. Under sufficiently restrictive conditions on the potential, these can be exactly identified with the poles of the scattering matrix. Here, that proof will not be given.

5.0.2 Analyticity of eigenfunctions

All energies in the point spectrum (bound states and resonances) are associated with eigenfunctions. As a consequence of analyticity, the projectors onto those eigenfunction are also analytic functions. The proof for this goes through the analyticity of the resolvent and the Riesz-projectors: integrals over analytic functions, if they exist, are analytic functions themselves, i.e.

$$\int_{C_b} dz (H_\theta - z)^{-1} = 2\pi i \Pi_{b,\theta}$$

(241)

Actually, can hope that also the eigenfunctions will be analytic functions. In the case of the hydrogen atom, this is quite obvious: the (radial) solutions have the form

$$Q_n(e^\lambda r) \exp(-\kappa_n e^\lambda r),$$

(242)

with some (Laguerre-type) polynomial $Q_n$. This is trivially analytic in $\lambda$.

On the real axis, the projector onto a scaled bound state is

$$\Pi_{n,\lambda} = |\Phi_{n,\lambda}\rangle \langle \Phi_{n,\lambda}|.$$  

(243)

In the complex plane, one has to consider that complex conjugation is not an analytic map. For s.a. Hamiltonians, eigenfunctions can be chosen as real such that the only source of imaginary parts will be the complex
scaling. The corresponding imaginary parts should \textit{not} change signs, such that the complex continued projector is

\[ \Pi_{n,\theta} = |\Phi_{n,\theta}\rangle \langle \Phi_{n,\theta}^*|, \tag{244} \]

i.e. the bra-vector is used without complex conjugation. More generally, one can write this by observing that an operator and its adjoint will share spectral values, but have different left and right eigenvectors:

\[ \Phi_L \neq \Phi_R : \quad H|\Phi_R\rangle = |\Phi_R\rangle E, \quad H^\dagger|\Phi_L\rangle = |\Phi_L\rangle E^* \tag{245} \]

and write

\[ \Pi_{n,\theta} = |\Phi_{R,n,\theta}\rangle \langle \Phi_{L,n,\theta}|, \tag{246} \]

5.1 The origin of resonances

Resonances can arise from a range of contexts. One example can be seen in scattering at a potential well, as discussed in the context of the Ramsauer-Townsend effect: where the phase shift of the partial wave across the potential reaches \( \delta_l(k) = (2n + 1)\pi/2 \), we will see a peak in the partial wave cross section \( \sigma_l(k) = 4\pi/k^2(2l + 1) \sin^2 \delta_l(k) \).

In many cases, the appearance of a resonance can be connected to a bound state of some “unperturbed” system. Here we discuss a few of these cases.

5.1.1 Fermi golden rule

A resonance is behind the famous “Fermi golden rule” for the lifetime of a state in presence of some matrix element connecting it to a continuum at the same energy. This is a standard textbook example, and it is usually derived using time-dependent perturbation theory. In fact, it is better described using stationary perturbation theory, using complex scaling to justify the result.

The FGR decay width in its simplest form is given by the square of the bound-continuum transition matrix element at the initial bound state energy \( E \):

\[ \Gamma = 2\pi|\langle E_0|V|\Phi_0\rangle|^2, \tag{247} \]
where \( \Phi_0 \) is the unperturbed bound state at energy \( E_0 \) and \( |E_0\rangle \) is the \( \delta \)-normalized continuum state at that energy. If the continuum at \( E_0 \) is degenerated we write

\[
\Gamma = 2\pi \sum \int d\alpha |\langle E_0, \alpha | V | \Phi_0 \rangle|^2. \tag{248}
\]

In literature, you usually find a “density of states” \( \rho(E) \) included, which accounts for the proper \( \delta \)-normalization and also for degeneracy in cases, where all \( \alpha \) have the same matrix element.

A generic Hamiltonian that can be associated with FGR is

\[
H = H_0 + V \tag{249}
\]

\[
H_0 = |\Phi_0\rangle E_0 \langle \Phi_0 | + \int_0^\infty dE \sum \int d\alpha |E, \alpha \rangle E \langle E, \alpha |
\tag{250}
\]

\[
V = \int_0^\infty dE \sum \int d\alpha [|E, \alpha \rangle v(E, \alpha) \langle \Phi_0 | + h.c.], \tag{251}
\]

and \( E_0 > 0 \): it is important, that \( E_0 \) is equal to one of the continuum energies \( E \).

If \( V \) is weak, we may try to apply standard perturbation theory (for notational simplicity we drop degeneracy of the continuum states). The first correction is \( E_0^{(1)} = \langle \Phi_0 | V | \Phi_0 \rangle \). Second order would be

\[
E_0^{(2)} = \int dE \frac{\langle E | V | \Phi_0 \rangle|^2}{E - E_0} = \langle \Phi | V \Pi_\perp (E_0 - H_0)^{-1} \Pi_\perp V | \Phi \rangle. \tag{252}
\]

In the second form, we have defined the projector

\[
\Pi_\perp = 1 - |\Phi_0\rangle \langle \Phi_0 |, \tag{253}
\]

which removes the unperturbed state from the resolvent. The expression is reminiscent of a second Born amplitude of the \( T \)-matrix, and it shares its problem, viz. that the resolvent is singular at \( E = E_0 > 0 \). A seemingly \textit{ad hoc} remedy is to add a \( -i\epsilon \) to the denominator and approach \( E_0 \) from the complex plane.

We obtain an imaginary part to of \( E_0^{(2)} \) as

\[
\Im m \lim_{\epsilon \downarrow 0} \frac{1}{E + i\epsilon - E_0} = -\pi \delta(E - E_0) : \tag{254}
\]

with this, the imaginary part is just 1/2 of the FGR decay width.

A justification for this follows in the next subsection.
Doubly excited states and Feshbach resonances

The generic Hamiltonian (249) can be made specific by choosing the Helium atom as an example:

\[ H_0 = \sum_{i=1}^{2} -\frac{1}{2} \Delta_i - \frac{1}{r_i}, \quad V = \frac{1}{|\vec{r}_1 - \vec{r}_2|}, \]  

i.e. we treat the electron-electron interaction as a “perturbation”. The continuum of \( H_0 \) starts at \(-2au\), when one electron is unbound and the other is in the ionic ground state. Let us denote such a state as \( |E\rangle := |n = 1, k\rangle \), omitting all specifications of angular momentum for notational brevity. Any state where both electrons are in an excited ionic state, denoted as \( |\Phi_x\rangle = |n_1, n_2\rangle \), \( n_1, n_2 > 1 \) will have an energy \( E_x = E_1 + E_2 > -\frac{2}{n_1^2} - \frac{2}{n_2^2} \), i.e. \( E_x \) is immersed into the continuum of \( |E\rangle \)-states. In absence of \( V \), the electrons are unaware of their mutual existence and such a doubly excited state is strictly bound. As soon as there is any mechanism for the two electrons to exchange energy (i.e. \( V \)), one electron drops to the ground state and the other is promoted into the continuum: we have a non-vanishing matrix element

\[ \langle n = 1, k | V | \Phi_x \rangle \neq 0, \]  

which enters the FGR decay rate. Of course, one needs to question, whether a perturbative treatment is legitimate here, considering that the \( V \) raises the ground state binding energy from \( E_{th} - E_0 = -2 - (-4) = -2 \) for \( H_0 \) to the Helium ground state binding energy for \( H_0 + V \) with a value of 0.9037. Indeed FGR gives good values only when the two principal quantum numbers differ significantly. (This is easy to understand if we consider that the two electrons reside in different spatial regions and barely overlap.)

We can readily complex scale \( H_0 \) and also \( V \). The spectrum of the complex scaled \( H_{0,\theta} \) is the sum of the spectra of the two independent ionic Hamiltonians: at each bound state of one ionic Hamiltonian, the spectrum of the other ionic Hamiltonian is attached. The doubly excited bound states \( |\Phi_x\rangle \) are located between thresholds. We can now compute perturbative corrections to these bound states using \( \alpha V \), keeping \( \alpha \) sufficiently
small for now. Perturbation theory does not require operators to be self-adjoint. It is applicable whenever an energy is isolated from the rest of the spectrum.

The perturbative correction is

\[ E^{(2)}_{x,\theta} = \langle \Phi^*_{x,\theta} | V_{\theta} \Pi_{\perp,\theta} (H_{0,\theta} - E_x)^{-1} \Pi_{\perp,\theta} V_{\theta} | \Phi_{x,\theta} \rangle. \]  

(257)

Here, we do not need to add an \( i\epsilon \), is the resolvent is not singular at \( E_0 \) and perturbation theory remains directly applicable.

Again, we have \( E^{(2)}_{x,\theta} \) as an integral of a product of analytic functions, i.e. it is analytic. We can add an \( i\epsilon \) and compare the result for real scaling with the complex scaled result: it is constant for real scaling, therefore \( E^{(2)}_{x,\theta} \) coincides with the FGR result.

Of course, complex scaling provides also the exact, non-perturbative position \( E_{x,\theta} \) of the resonance: you can view as the original \( E_{x,\theta}^{(0)} \) pulled into the complex plain by the interaction with the complex continua in its vicinity. Note that \( E_{x,\theta} \) is independent of \( \theta \) as long as no continuum sweeps over it: it is invariant if we add a real part to the scaling parameter (i.e. unitary transformation), therefore invariant in a whole surrounding of the original \( \theta \).

In addition we can now associate a unique function from Hilbert space with it, let us call it \( \Psi_{x,\theta} \) and we can solve the eigenvalue problem for that in Hilbert space.

The generalization of this concept is the so-called Feshbach resonance: we have a few-body problem that exhibits an exact bound state immersed into a continuum, with which it does not interact in absence of perturbation. When a perturbation is added, the boundstate converts into a continuum and acquires an imaginary part. This is amply exploited in ultracold systems. There, an external handle (often a magnetic field) is introduced to manipulate the position of the resonance, in first approximation the bound state energy.

5.1.3 Fano theory

An interesting case is the theory of Fano resonances. This, basically, is a simple interference phenomenon. From our point of view, the interesting
thing is that the resolvent of model Hamiltonian and therefore the scattering amplitude and cross-section can be calculated exactly.

The Fano process is a transition from some bound state into a continuum which has a FGR-like resonance. Typically, a system in its initial state $|i\rangle$ would be excited to a continuum state $|E\pm\rangle$ by absorbing one photon with energy $\hbar\omega = E - E_i$. By $|E\pm\rangle$ we indicate that the continuum consists of non-trivial scattering states that are modified by the presence of an immersed resonance. The cross section for photo-absorption has a characteristic line shape

$$
\sigma(\Delta) = \sigma_0 \frac{|q\Gamma + 2\Delta|^2}{\Gamma^2 + (2\Delta)^2},
$$

where $\Delta$ parameterizes is the “detuning” of the energy $E$ from the resonance position $E_r$ and $q$ is the “Fano $q$-parameter”. At $\Delta = 0$ the cross-section peaks, and, depending on the sign of $q$ it dips to 0 at some positive or negative $\Delta$, i.e. above or below the resonance energy.

In lowest order of the photon-interaction, the cross section is given as

$$
\sigma(E) \propto |\langle E\pm | T |i\rangle|^2,
$$

where $T$ is the transition operator, typically the dipole operator $\vec{r}$. The characteristic Fano dip arises from the energy dependence of the continuum states $|E\pm\rangle$. These are the scattering solutions of a FGR-type Hamiltonian

$$
H =: H_0 + V = |0\rangle E_0 \langle 0| + \int dE |E\rangle E \langle E| + |v\rangle \langle 0| + |0\rangle \langle v|
$$

The dip in the line-shape can be understood as the destructive interference of a transition from the initial state $|i\rangle$ into the embedded bound state $|0\rangle$ that decays and a “direct” transition into the continuum states $|E\rangle$, which are considered as structureless, i.e. with weak $E$-dependence.

(further refer to fano-theory.pdf).

**Problem 5.26: The Woodbury formula** is a useful identity for the inverse of an operator of the form $A = A_0 + UMW^\dagger$:

$$
A^{-1} = A_0^{-1} - A_0^{-1}U \left[ W^\dagger A_0^{-1}U + M^{-1} \right]^{-1} W^\dagger A_0^{-1}
$$

Show this!
Problem 5.27: Fano states and profile

(a) Compute the Møller operator for

\[ H = H_0 + V = |0\rangle E_0 \langle 0| + \int dE |E\rangle E \langle E| + |v\rangle \langle 0| + |0\rangle \langle v|, \]

considering the last two terms as the V. Bound and continuum states of \( H_0 \) are orthogonal: \( \langle 0|E \rangle = 0 \). Explicitly take the limit \( \epsilon \downarrow 0 \). For the scattering solution, you should obtain

\[ |E_\pm\rangle = \frac{1}{E_0 + F(E) - E \pm i\pi|V(E)|^2} \times \left[ (E_0 + F(E) - E)|E\rangle - V(E)^* \left( |0\rangle + P \int dE'|E'\rangle V(E') E - E' \right) \right] \]

with

\[ P \int dE'|V(E')|^2 \left( \frac{E}{E - E'} \right) =: F(E), \quad V(E) := \langle E|v \rangle. \]

**Hint:** For computing the resolvent \((E - H \pm i\epsilon)^{-1}\) write \( H = H_0 + W\sigma_1 W^\dagger \) with \( W := (|0\rangle, |v\rangle) \) and \( \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \), then use the Woodbury formula. It can be useful to introduce short hand notation for the diagonal elements of the \( 2 \times 2 \)-matrix appearing in the Woodbury formula. Also note \( V|E\rangle = |0\rangle \langle v|E\rangle = |0\rangle V^*(E) \).

(b) Show

\[ \langle E_-|T|I\rangle \propto \frac{1}{\pi|\langle 0|V|E\rangle|} \Phi(E) \langle E|T|I\rangle \sin \Delta - \langle E|T|I\rangle \cos \Delta \]

with

\[ \Delta(E) = -\arctan \frac{\pi|\langle E|V|0\rangle|^2}{E - E_0 - F(E)}, \]

and the resonant contribution \( \Phi(E) \).
6 Multi-channel scattering

6.1 Inelastic scattering

So far we have assumed that there is only a single particle and no internal structure of the scatterers. In reality, scattering may proceed in-elastically. Imagine a positron scattering from an atom: it will interact with the atom’s electron and, in principle, it can put the atom into an excited state. (We choose a positron rather than an electron to avoid questions arising with indistinguishable particles.) How can we describe this situation in the framework of $S$-matrix theory?

As the simplest model, assume our target is a two-level system, which can be put from the ground into the lowest excited state, but we exclude excitation to higher excited states or ionization. Let

$$H_c = \int d^3k |\vec{k}, c\rangle (k^2/2 + E_c) \langle \vec{k}, c|, \quad c = g, x$$

be the Hamiltonians for free positron and the atom in the ground and excited states, respectively. The states $|\vec{k}, c\rangle = |\vec{k}\rangle \otimes |c\rangle$ describe a free positron with momentum $\vec{k}$ and the atom in state $c = x$ or $g$.

$E$ is the total energy, $E_g$ and $E_x$ are the ground and excited state energies of the atom, and $E - E_c$ is the energy of the positron scattering in “channel” $c$.

We write a scattering potential in the form

$$H_I = \int d^3k \int d^3k' \delta(k' - k) \left[ |\vec{k}, g\rangle V_{gg} \langle \vec{k}', g| + |\vec{k}, x\rangle V_{xx} \langle \vec{k}', x| \right] + \delta(k' - q(k)) \left[ |\vec{k}', x\rangle V_{xg} \langle \vec{k}, g| + |\vec{k}, g\rangle V_{gx} \langle \vec{k}', x| \right].$$

with $q(k) = \sqrt{k^2 + 2E_g - 2E_x}$ and integration ranges are adjusted such that the argument of the root remains $\geq 0$.

The first line describes elastic scattering processes where the atom remains in $|g\rangle$ or $|x\rangle$ and the second line generates transitions from the ground to excited state and back. The total Hamiltonian is

$$H = H_g + H_x + H_I$$

Note that the $S$-matrix formalism does not make any assumptions about the exact nature of the Hamiltonians involved. The only assumption is
that at long times the time-evolutions by \( H_0 \) and \( H \) become equal. Thus we choose for the comparison Hamiltonian \( H_0 \)
\[
H_0 = H_g + H_x
\]
and the scattering “potential” \( V \) is
\[
V := H_f.
\]

The \( V_{cc'} = \langle \vec{k}, c | V | \vec{k}', c' \rangle \) are functions of \( \vec{k} \) and \( \vec{k}' \).

The concept of scattering cross section must be extended to include the fact that the atom can be either in its ground state \( |g\rangle \) or in the excited state \( |x\rangle \). For each pair of channels \( c = g \) or \( x \) and \( c' = g \) or \( x \), we define a scattering cross section as follows. Assume you have an incident beam of electrons that hits the atom in the state state \( |c\rangle \). What is the probability of finding in the scattered wave packet the atom in the state \( |c'\rangle \) in the energy range \( \Delta E \)?

The procedures are essentially the same as for a single particle.

- Set up a normalized incident wave packet, preferably with the atom in either state \( |g\rangle \) or \( |x\rangle \).
- Write down the probability for finding a given final range of final positron momenta and atomic state \( |g\rangle \) or \( |x\rangle \).
- Average over all impact parameters keeping the number of particles per surface unit constant, i.e. do the integral \( \int_{\mathbb{R}^2} d(2)a \).
- Handle the \( \delta \)-functions. Here arises a new feature as total energy \( E = k^2/2 + E_c \) is conserved, but not the energy of the scattering positron alone \( k^2/2 \). This adds a factor \( k/k_0 \) to our equation.

In this way one finds for the channel scattering cross section
\[
\frac{d\sigma_{cc_0}}{d\Omega} = \frac{k}{k_0} |f_{cc_0}(\vec{k}, \vec{k}_0)|^2
\]
with
\[
f_{cc_0}(\vec{k}, \vec{k}_0) = -(2\pi)^2 \langle \vec{k}, c | V_c + V_c(\frac{k^2}{2} + E_c - H + i\epsilon)^{-1}V_c_0 | \vec{k}_0, c_0 \rangle
\]
Where $V_c := H - H_c$. Note that because of conservation of total energy $E = k^2 + E_c = k_0^2 + E_{c0}$

\[
\langle \vec{k}, c | V_{c0} | \vec{k}_0, c_0 \rangle = \langle \vec{k}, c | H - H_{c0} | \vec{k}_0, c_0 \rangle = \langle \vec{k}, c | H - E | \vec{k}_0, c_0 \rangle \quad (270)
\]
\[
= \langle \vec{k}, c | H - E | \vec{k}_0, c_0 \rangle = \langle \vec{k}, H_{c}c | V_c - E | \vec{k}_0, c_0 \rangle \quad (271)
\]
\[
= \langle \vec{k}, c | V_c | \vec{k}_0, c_0 \rangle \quad (272)
\]

**Post and prior forms:** In this case the distinction between the “post” and “prior” forms of the scattering amplitude becomes relevant. We can write the

\[
f(\vec{k}, \vec{k}_0) = -(2\pi)^2 \langle \vec{k}, c | V_c | \Psi_{c0}^- (\vec{k}_0) \rangle \quad \text{“post” form} \quad (273)
\]
\[
= -(2\pi)^2 \langle \Psi_c^+ (\vec{k}) | V_{c0} | \vec{k}_0, c_0 \rangle \quad \text{“prior” form} \quad (274)
\]

and each of the two forms may allow different approximations, depending on the exact shape of $V_c$ and $V_{c0}$ or the scattering waves $\Psi_c^{(\pm)} (\vec{k})$. E.g. one of the channels may have very high or very low scattering energy, which makes replacing the scattering wave function by plane waves seem more legitimate.

6.1.1 S-matrix

The $S$-matrix for this inelastic scattering is

\[
S = \Omega_+^\dagger \Omega_-.
\]

In potential scattering the $S$ matrix conserved asymptotic energy of the free particle $k^2/2$ and we could represent it as a function of $k$. We need, in addition the asymptotic kinetic energy also the bound state energy. Matrix elements of the $S$ matrix will therefore depend on $k$ as well as on the integral state before and after the scattering:

\[
S = \begin{pmatrix} S_{gg} & S_{gx} \\ S_{xg} & S_{xx} \end{pmatrix}.
\]

6.1.2 LS-equation

Generalization for inelastic scattering is straight forward:

**Problem 6.28:** Multi-channel LS-equation
• Derive

$$|\psi^{(\pm)}_{c,\vec{k}}\rangle = |\vec{k}, c\rangle - (H_c - E \pm i\epsilon)^{-1}V_c|\psi^{(\pm)}_{c,\vec{k}}\rangle$$

with $V_c = H - H_c$ for the inelastic case.

**Hint:** Start from the LS equation for the full problem and identify the $c$-component.

• Show that the same form applies for general multi-channel scattering.

**Hint:** Start from the definition of $\Omega^{(a)}_\pm$ and observe that the stationary form ($\epsilon$-limit) is the exact same as in potential scattering.

Above, we were able to trivially solve scattering problem for $H_c$ and therefore we were able to use $(H_c - k^2/2 \pm i\epsilon)^{-1}$ in the spectral amplitude. In more realistic problems, already solution of the channel problem may pose a problem.

**Problem 6.29: Multi-channel Born approximation** Write the multi-channel LS-equation in first Born approximation w.r.t. $H_\alpha$. Rewrite $(H_\alpha - E \pm i\epsilon)^{-1}$ using the (exactly known) $(-\Delta/2 - E \pm i\epsilon)^{-1}$ and the Møller operators $\Omega^{(a)}_\pm$. Approximate the Møller operators by the first two terms of the resolvent series and consider the result up to first and second order of potentials.

### 6.1.3 An alternative view

We will now formalize the expectation

$$S_{cc'} = (\Omega^{(c)}_+ \Omega^{(c')}_-), \quad c, c' \in \{g, x\}$$

Above we have used the formalism exactly as developed so far, as a comparison between two time evolutions $H_0$ and $H$, where

$$H_0 = -\frac{1}{2}\Delta \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

(279)

describes free motion with the scatterer in either $g$ or $x$.

and the Møller operators

$$\Omega^{(c)}_\pm = \lim_{t \to \pm \infty} \exp(-itH) \exp(itH_0) P_c.$$ (280)
Here we have added a projector
\[ P_g = 1 \otimes \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad P_x = 1 \otimes \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \] (281)
that admits only asymptotic states in the respective channel.

The channel Hamiltonians commute \([H_c, H_{c'}] = 0\) and therefore the two asymptotic subspaces are (rather trivially) orthogonal
\[ P_c P_{c'} = \delta_{cc'} P_c. \] (282)

\(H_0\) is a sum of the channel Hamiltonians \(H_c\):
\[ H_0 = H_g P_g + H_x P_x \] (283)

Similarly
\[ \Omega_\pm = \Omega_{\pm}^{(g)} + \Omega_{\pm}^{(x)} \] (284)
and we can read off the scattering matrix elements (278).

6.1.4 Distorted waves

We are free to choose the alternative comparison Hamiltonian
\[ \tilde{H}_0 = \sum_c \tilde{H}_c = \sum_c -\frac{1}{2} \Delta + \int d(3) k |k, c\rangle V_{cc} \langle k, c|, \] (285)
assuming that we either can exactly solve or independently approximate the scattering problem for \(\tilde{H}_c\).

6.2 Two interacting particles in a potential

In inelastic scattering we could essentially straight forwardly extend the theory of potential scattering. However, the general multi-particle case shows fundamental complications due to the fact the spaces \(H_{ac}(H_a)\) may not be orthogonal.

The simplest system that shows all complications are two particles in a potential that interact by a force \(V_I\). Assume all forces are short range. The Hamiltonian on \(L^2(\mathbb{R}^3) \otimes L^2(\mathbb{R}^3)\) (with proper domain, not essential for this discussion) is
\[ H(1, 2) = H_1 \otimes 1_2 + 1_1 \otimes H_2 + V_I(1, 2) \] (286)
where $H_1$ and $H_2$ are Hamiltonians on $L^2(\mathbb{R}^3)$ and $V_I(1, 2)$ is a multiplication operator on $L^2(\mathbb{R}^3) \otimes L^2(\mathbb{R}^3)$, say with kernel
\[ V(\vec{x}_1 - \vec{x}_2). \] (287)

There are several different asymptotic situations

- (012) \ldots all particles bound, state in the point spectrum of $H$
- (01)+2 \ldots 1 bound, but 2 free, state in the continuous spectrum $\sigma_c(H)$, but 1 in the bound spectrum $\sigma_p(H_1)$
- (02)+1, 1 ↔ 2 of the above
- (12)+0 \ldots 1 and 2 bound by $V_I$
- ()+0+1+2 \ldots both particles free

To specify the asymptotic situation fully, we must for each case define the asymptotic bound state (if any), say $|a\rangle := \psi_n^{(ij)}$ where $n$ labels the bound states of $(ij) = (01), (02), (12)$. $a$ designates the asymptotic channel. The comparison Hamiltonian for channel $a$ is then
\[ H_\alpha = -\Delta_\alpha \otimes \sum_a |a\rangle E_a \langle a| \] (288)

where $\alpha$ denotes the coordinates from the center-of-mass of particles $i$ and $j$ to the remaining particle and
\[ -\frac{1}{2m_{ij}} \Delta_{ij} + V(\vec{r}_i - \vec{r}_j)|a\rangle = |a\rangle E_a, \] (289)

with the reduced mass of particles $i$ and $j$. For simplicity, we have assumed particle 0 as infinitely heavy. If this is not the case, appropriated reduced masses need to be used.

In addition there is the breakup channel $\alpha = ()$ with the channel Hamiltonian.
\[ H() = -\frac{1}{2m_1} \Delta_1 - \frac{1}{2m_2} \Delta_2. \] (290)

We identify a channel as subset of coordinates w.r.t. to which all particles remain bound and the (appropriately constructed) remaining coordinates, where the motion is free.
The construction of a single wave operator "$e^{itH}e^{-itH_0}$" to describe all these situations is not possible, since there is no single $H_0$ that can describe all channels simultaneously. We can readily give the projectors $P_\alpha$ onto $\mathcal{H}_{ac}(H_\alpha)$

$$P_\alpha = 1_\alpha \otimes \sum_a |a\rangle \langle a|, \quad P() = 1, \quad P_{(012)} = 0. \quad (291)$$

The $ac$ spectral spaces $P_{ac}(H_\alpha)\mathcal{H}$ are not mutually orthogonal. Simplest to see by looking at the total breakup $0 + 1 + 2$ with $H()$, whose $ac$-spectrum spectral subspace is the whole $L^2(\mathbb{R}^3) \otimes L^2(\mathbb{R}^3)$, while obviously any other channel is part of that: $P_{(ij)}P() = P_{(01)}$. So, if we cannot decompose the initial wave packet uniquely into components $P_{ac}(H_\alpha)\mathcal{H}$, for which $H_\alpha$ should we compute the Møller operators and the scattering wave packet $\Psi^{(\pm)}$?

The solution is that, the if the channel Møller operators

$$\Omega^{(\pm)}_\alpha := \lim_{t \to \pm \infty} e^{itH}e^{-itH_\alpha}P_\alpha \quad (292)$$

exist, one can show that they map onto mutually orthogonal subspaces of $\mathcal{H}_{ac}(H)$.

That means that while a given wave-packet cannot be unambiguously decomposed into contributions belonging to a given channel from its behavior in the remote past (alternatively: remote future) alone, the scattering wave packets

$$\Psi^{(\pm)}_\alpha = \Omega^{(\pm)}_\alpha \phi, \quad \phi \in \mathcal{H} \quad (293)$$

are orthogonal:

$$\langle \Psi^{(\pm)}_\alpha | \Phi^{(\pm)}_\beta \rangle = 0 \text{ for } \alpha \neq \beta. \quad (294)$$

We can uniquely decompose the corresponding scattering wave packet into scattering (not channel) contributions with the respective asymptotic behavior. We need the information of the actual scattering process for resolving the ambiguity contained in the asymptotic behavior alone. This is different here from the case of inelastic scattering, where the asymptotics could be unambiguously related to a given Hamiltonian and therefore be decomposed into "incoming ground" or "incoming excited" channels etc. without any reference comparison to the actual scattering.
The physical reason for this orthogonality is that, by construction, \( \alpha \neq \beta \) implies that the two channels differ in at least one coordinate, where, say, \( \alpha \) would be bound, but \( \beta \) is free. Wave packet spreading of free motion (i.e. \( \Phi_\beta(t) \to 0 \)) while \( \Psi_\alpha(t) \) remains localized w.r.t. to the same coordinate. That implies that the overlap of \( \beta \) with the \( \alpha \) w.r.t. to that coordinate \( \to 0 \).

Let us consider the channels \( \alpha = (01) \) and \( \beta = (02) \) in our present example. We have assumed that the channel Møller operators exist a strong limits, i.e.

\[
\lim_{t \to \pm \infty} e^{-itH} e^{itH_\alpha} P_\alpha \phi - \Omega_\pm^{(\alpha)} \phi = 0 \forall \phi \in \mathcal{H}.
\] (295)

From this follows

\[
||Q_\pm^{(\alpha)}\phi||^2 = \lim_{t \to \pm \infty} \langle \Omega_\alpha(t)\phi | \Omega_\alpha(t)\phi \rangle =
\]

\[
= \lim_{t \to \pm \infty} \langle e^{-itH} e^{itH_\alpha} P_\alpha \phi | e^{-itH} e^{itH_\alpha} P_\alpha \phi \rangle = ||P_\alpha \phi||^2
\]

and similarly

\[
[Q_\pm^{(\alpha)}]^2 = Q_\pm^{(\alpha)}
\] (296)

Note that although \( P_\alpha \neq Q_\alpha \), the norms agree for all \( \phi \): the difference between them is an isometric map from \( \mathcal{H}_{ac}(H_\alpha) \) to \( \mathcal{H}_{ac}(H) \). In more physical terms it can be understood such that for \( Q_- \alpha \) at some point in the remote past the norms agree. As the Møller operators are time-invariant also the \( Q_-^{(\alpha)} \) are, therefore the norms always agree. For \( Q_+^{(\alpha)} \), use the agreement in the remote future.

For our two channels we can write the Hamiltonians as

\[
H_{(01)} = -\frac{1}{2} \Delta \otimes \sum_a |a \rangle \langle a |, \quad H_{(01)} = \sum_b |b \rangle \langle b | \otimes -\frac{1}{2} \Delta,
\] (297)

where \( a \) and \( b \) run over all bound states of the (01) and (02) coordinate, respectively.

\[
\langle \Omega_\pm^{(\alpha)} \phi | \Omega_\pm^{(\beta)} \phi \rangle = \lim_{t \to \pm \infty} P_\alpha \phi | e^{-itH_\alpha} e^{itH_\beta} P_\beta \phi \rangle := \lim_{t \to \pm \infty} \langle \phi_\alpha | e^{-itH_\alpha} e^{itH_\beta} \phi_\beta \rangle
\]
For showing the orthogonality it is sufficient to show that $e^{-itH_\alpha}e^{itH_\beta} \to 0$:

$$\left[ \sum_a |a\rangle e^{-itE_a} \langle a| \otimes e^{-it\Delta/2} \right] \left[ e^{-it\Delta/2} \otimes \sum_b |b\rangle e^{-itE_b} \langle b| \right] =$$

$$\left[ \sum_a |a\rangle e^{-itE_a} e^{-it\Delta/2} e^{-it\Delta/2} \langle a| \right] \otimes \left[ e^{-it\Delta/2} \sum_b |b\rangle e^{-itE_b} \langle b| \right]$$

Now, to the separate tensor factors, the wave-packet spreading argument applies. (If you like: RAGE theorem). Similar reasoning can be carried through for all partitionings.

Mutual orthogonality of the images of $\Omega_\pm^{(\alpha)}$ means

$$(\Omega_\pm^{(\alpha)})^\dagger \Omega_\pm^{(\beta)} = \delta_{\alpha\beta} P_\alpha.$$  \hspace{1cm} (298)

We remember that

$$\Omega_\pm^{(\alpha)} : \mathcal{H}_{ac}(H_\alpha) \to \mathcal{H}_{ac}(H)$$  \hspace{1cm} (299)

The map is no longer surjective, i.e. on to all of $\mathcal{H}_{ac}(H)$, but onto a subspace. The projector onto that subspace can be constructed: As the image of, say, $\Omega_\pm^{(\alpha)} \subset \mathcal{H}_{ac}(H)$ and the Møller operators do not change the norm when considered as maps from $\mathcal{H}_{ac}(H_\alpha)$, the operators

$$Q_\pm^{(\alpha)} := \Omega_\pm^{(\alpha)} (\Omega_\pm^{(\alpha)})^\dagger$$  \hspace{1cm} (300)

are projectors onto the respective subspaces of $\mathcal{H}_{ac}(H)$. Orthogonality of these subspaces means that

$$Q_\pm^{(\alpha)} Q_\pm^{(\beta)} = \delta_{\alpha\beta} Q_\pm^{(\beta)}.$$  \hspace{1cm} (301)

Note that

$$Q_-^{(\alpha)} \neq Q_+^{(\alpha)}$$  \hspace{1cm} (302)

in general, the two projectors differ. For a given channel $\alpha$, it matters whether we construct the subspace by going back or forward in time. It is easy to understand on physical grounds why this cannot be: suppose we have an incoming state in the channel $\alpha = (01)$ channel, i.e. particle 1 bound. In the reaction, all three channels can be generated: $(01), (02), ()$. If we want to create that scattering state by going into the remote future, we need components in all three channels, not just in the original $\alpha = (01)$.
Of course, the two scattering state subspaces are related by time-reversal:

\[ Q^{(\alpha)}_+ = KQ^{(\alpha)}_- K, \]  

(303)

if \( K \) denotes the time-reversal operator.

### 6.2.1 Asymptotic completeness

For the few-body situation completeness means that, going through all possible channels \( \alpha \), we can build all scattering states in \( \mathcal{H}_{ac}(H) \). That means all \( Q^{(\alpha)}_+ \) (or \( Q^{(\alpha)}_- \)) together project onto the complete \( ac \) spectral subspace of \( H \)

\[ \sum_{\alpha} Q^{(\alpha)}_\pm \mathcal{H} = P_{ac}(H)\mathcal{H}. \]  

(304)

### 6.2.2 Jacobi-coordinates

With different clustering of particles (01), (02), (12), the choice of coordinates is not necessarily obvious: with an infinite mass for particle 0, the coordinates

\[ \vec{r}_{01} = \vec{r}_1 - \vec{r}_0, \vec{r}_{02} = \vec{r}_2 - \vec{r}_0 \]  

(305)

are natural choices. Already in the (12) channel, it is advisable to choose the relative coordinates

\[ \vec{r}_{12} = \vec{r}_2 - \vec{r}_1 \]  

(306)

and the coordinate from \( \vec{r}_0 \) to the center-of-mass of (12):

\[ \vec{r}_J = \frac{m_1 \vec{r}_1 + m_2 \vec{r}_2}{m_1 + m_2} - \vec{r}_0. \]  

(307)

This is the simplest form of “Jacobi coordinates” which connect the centers-of-masses of a hierarchy of sub-clusters. Only with such coordinates, the channel Hamiltonians factor in the simple shape that we used. We could conveniently use the fact that for the channels (01) and (02), the Hamiltonians factorize into tensor products with respect to the same tensor factors

\[ \mathcal{H} = L^2(\mathbb{R}^3, \vec{r}_1) \otimes L^2(\mathbb{R}^3, \vec{r}_2) \]  

(308)

with kinetic energy in the unbound channels in the form \(-\Delta\).
Already at finite mass for particle 0, we lose that convenience. In that case we can either keep the factorization (308), but than obtain contributions to kinetic energy terms that of the form
\[ \vec{\nabla}_1 \otimes \vec{\nabla}_2, \] (309)
sometimes called “mass polarization terms”.

Alternatively, we can choose Jacobi coordinates in all channels and the corresponding reduces massed for the energy. This is the standard choice for abstract scattering theory, as it simplifies the discussion of free motion.

Already with three particles, the choice of Jacobi coordinates is not unique for the \( \alpha = () \) channel, as the sequence of grouping the particles is not unique, one for each pair-wise clustering (ij).

6.2.3 The \( S \)-matrix (interaction picture)

This is what we have discussed so far, a map from one channel \( \beta \) where particles are bound w.r.t. to the subset of coordinates \( \beta \) and free for the rest into channel \( \beta \):
\[ S_{\alpha\beta} = \Omega_+^{(\alpha)} \Omega_-^{(\beta)}. \] (310)

6.2.4 The \( S \)-matrix (Heisenberg picture)

Problem 6.30: \( S \)-matrix in the Heisenberg picture

One can define an \( S \)-matrix as
\[ S = \sum_{\alpha} \Omega_-^{(\alpha)} (\Omega_+^{(\alpha)})^\dagger. \] (311)

(a) On which subspace(s) does \( S \) operate?

(b) Show that \( \Omega_+^{(\alpha)} (\Omega_-^{(\alpha)})^\dagger \Psi^{(-)}_{\beta, k} = \delta_{\alpha\beta} \Psi^{(+)}_{\alpha, \vec{k}}. \)

(c) Show that \( S \) is related to \( S_{\alpha\beta} \) by
\[ \langle \vec{k}, \alpha | S_{\alpha\beta} | \vec{k}', \beta \rangle = \langle \Psi^{(-)}_{\alpha \vec{k}} | S | \Psi^{(-)}_{\beta \vec{k}'} \rangle. \]

(d) Assuming asymptotic completeness, show that \( S \) is unitary on \( \mathcal{H}_{ac}(H) \).
The $S$ of the Heisenberg picture has the virtue of being unitary which $S_{\alpha\beta}$ is not, as it maps between different subspaces. For using it in practice, one needs access to the scattering functions $\Psi_{\alpha,\vec{k}}^{(\pm)}$.

6.3 Graphical representation of the resolvent

With the resolvent playing the lead role in scattering, the resolvent equation, its extension to multi-channel, and expansion into a series (as in the Born-series) play a central role. This is, in fact, what is behind the popular Feynman diagrams with their intuitive physical interpretation.

Resolvents are linear operators (and bounded), therefore one can add and multiply them: they form an algebra. As we only want to make you aware of this formally, we do not discuss questions of convergence of a series.

Also, there are certain elements of choice in using the resolvent formula: we may subsume parts of the interaction into the resolvent. The Kohn variational principle was an example where one isolates a solvable part and remains with a correction, that can be neglected or be treated approximately.

Let us remain with our 3-particle problem, but adjust notation for the purpose

$$H = T + v_1(\vec{r}_1 - \vec{r}_0) + v_2(\vec{r}_2 - \vec{r}_0) + v_3(\vec{r}_2 - \vec{r}_1)$$  \hspace{1cm} (312)

then we can use the resolvent series to first, e.g., expand

$$\frac{1}{z - H} = \frac{1}{z - (H - v_1) - v_1} = \frac{1}{z - (H - v_1)} \sum_{n=0}^{\infty} \left[ v_1 \frac{1}{z - (H - v_1)} \right]^n$$  \hspace{1cm} (313)

and repeat the process for $[z - (H - v_1)]^{-1} = [z - (H - v_1 - v_2) - v_2]^{-1}$, etc. We end up with a multiple sum of the form $(R_0 := (z - T)^{-1})$

$$\frac{1}{z - H} = \sum_{n=0}^{\infty} \sum_{\gamma_1=1}^{3} \cdots \sum_{\gamma_n=1}^{3} R_{0\gamma_1} R_{0\gamma_2} \cdots R_{0\gamma_n}$$  \hspace{1cm} (314)

which we have sorted by powers of $R_0$. This is clearly a rather large sum and proper book keeping of all terms is needed. We do this by introducing the graphical notation:

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Absorbing part of the interaction into the resolvents amounts to not carrying the expansion to the point where all $R_0$ are free motion, but rather include the effect of, say, an external potential by using some $R_x$ instead of $R_0$. In the corresponding graphics, one can distinguish this by a different kind of line, e.g. fat.

A typical and extensively used example of such a corrected resolvent is the “self-energy” correction. The terms missing to the full resolvent are then, more often than not, neglected altogether.

### 6.3.1 Example

The importance of this is, however, not only a matter of book-keeping. The symbols can be distinguished into those that do involve an interaction between them (or to the outside, the infinitely heavy nucleus), and those that are connected. It turns out that operators corresponding to connected graphs are compact (like, e.g. $(p^2 - z)^{-1}V$ for a single particle). We had used several times, that such “relatively compact” operators leave the continuous spectrum unchanged, which is obviously an important property for scattering problems. The graphical representation allows to easily distinguish the compact parts from the non-compact. In our example, we draw:

where we have collected disconnected parts as
And finally cast this into a formula (Weinberg-Van Winter):

\[ R = D + JR = \text{(non-compact, spectrum known)} + \text{(compact) } R. \] (315)

As it holds that \((\text{compact}) \times (\text{bounded}) = \text{(compact)}\), we know that the continuous spectrum for \(R\) is the same as the continuous spectrum for \(J\). The latter is known and thus we know the spectrum for \(R\).
The Møller operators for the pair $H = -\Delta/2 - 1/r$ and $H_0 = -\Delta/2$ do not exist, which renders useless, at first glance, the instruments developed so far. There are several ways out of this predicament, each with its own merits and drawbacks. First, any truncation of the potential at a remote distance will alleviate the problem. Second, we actually know the exact (although a bit unwieldy) scattering solutions for the Coulomb problem. Thirdly, for the same reason that we know the exact solutions, we also can obtain the relevant scattering information without ever computing the scattering wave functions. Finally, we may choose for the comparison Hamiltonian $H_0$ into something for that the Møller operators do exist and whose spectral representation we still know.

### 7.1 Failure of standard scattering theory

An abstract way how the failure manifests itself is the fact that

$$\lim_{t \to \pm \infty} e^{it\Delta/2 + 1/r} e^{-it\Delta/2} = 0,$$

which means, as strong convergence would imply weak convergence, that we would obtain $\Omega_\pm = 0$, certainly not a suitable operator to obtain asymptotic completeness.

The problem is fundamental and easy to understand. Consider the classical motion on a trajectory that directs radially away from an attractive Coulomb potential $-1/r$. At radius $r$ and given total energy $E$, the classical momentum is $\sqrt{2E + 2/r}$. We also know that the velocity is bounded, therefore the position cannot grow more than linearly in time,

$$r(t) = ct + O(t).$$

Using this we see

$$\frac{1}{\sqrt{2}} \frac{d}{dt} r = \sqrt{E} \left[ 1 + \frac{1}{Ect + O(t)} \right] \approx \sqrt{E} \left[ 1 + \frac{1}{2Ect} + O(t^{-1}) \right]$$

where the expansion becomes valid where potential energy is only a small part of of total energy.
We find that the particle never moves like a free particle:

\[ r(t) \sim ct + d \log t. \]  

(319)

For attractive potentials, it will always “outrun” the free particle by any distance. Embarrassingly, our concept of scattering as comparing to free time-evolution fails fundamentally for this well-studied problem.

The slightly paradoxical impression that an attractive potential seems to cause the particle to move faster is readily dissolved when remembering that, at given asymptotic energy \( E \), the kinetic energy in an attractive, i.e. negative potential is higher than \( E \).

7.2 Compare to a different time-evolution

We will assert below that a meaningful asymptotic momentum exists for the Coulomb potential. This motivates the construction of comparison time-evolution that is based only on momentum, but differs from free motion. Such a Hamiltonian was proposed by Dollard

\[
H_D(t) = -\Delta - \frac{1}{2|t|\sqrt{-\Delta}} \theta(-4|t|\Delta - 1)
\]

(320)

and it turns out

\[
\Omega^{(D)}_\pm = \text{s- lim}_{t \to \pm \infty} e^{it(-\Delta-1/r)} e^{-i \int_0^t H_D(s)ds}
\]

(321)


The functions of \( \Delta \) are well defined, consider a momentum representation, and we know the eigenfunctions. An important drawback is that we cannot use the formulae of stationary scattering theory because of the time-dependence of \( H_D(t) \). This may be the reason why such techniques have found little practical application.

7.3 Asymptotic constants

From the above we learn, that the requirements of the beautiful apparatus of scattering theory are too strict: the exact comparison of the time-evolution is not what we usually seek. Instead, we want to know in which
direction (from some microscopic center) and at which momentum/energy a fragment arrives. Scattering theory where it exists, also requires, that motion towards the detector is essentially free: but this is not the case for Coulomb. When we do not require that, we can ask for “asymptotic observables”, i.e. observables that become constant at “infinite time” and at “infinite distance”, i.e. when we actually measure at our detector.

In strict terms, an asymptotic constant $A_\pm$ is the (strong) limit

$$\lim_{t \to \pm \infty} e^{-itH} Ae^{itH} = A_\pm$$

I.e., at sufficiently large times and for a given wave packet, the observable does not change any more. As always, the limit can work only in the strong sense, i.e. on a wave-packet wise level. Imagine momentum, which, we expect, will become constant eventually in a scattering process. But for (arbitrarily) slow fragments will take (arbitrarily) long time to leave the region of non-zero potential, and there will be no time when all, including the slowest, momenta have already assumed there final values within some preset $\epsilon$.

Of course, any conserved observable $[A, H] = 0$ is also an asymptotic constant, e.g. angular momentum $A = L^2$. The non-obvious constants of motion for the Coulomb potential are, as we would hope, momentum, direction, and the Coulomb potential itself, if we restrict them to the ac spectrum by the projector $P \mathcal{H} = \mathcal{H}_{ac}(H)$:

$$\lim_{t \to \pm \infty} (P \vec{p} P, \frac{\vec{r}}{|\vec{r}|} P, P \frac{1}{r} P) = (\vec{p}_\pm, \pm \frac{\vec{p}_\pm}{|\vec{p}_\pm|}, 0)$$

The sign of $\pm \vec{p}_\pm / |\vec{p}_\pm|$ reflects time-reversal: for the same value of momentum, we find a particle at negative times in the opposite direction from positive times. This expected result can be proven rigorously, but the proof involves surprisingly much effort.

For us, the message is: in the Coulomb problem, the momentum does assume a constant value asymptotically, although there is never strictly free motion. In that sense, the Coulomb force does become negligible at large distances.
7.4 Complete solution of the Coulomb problem

The high symmetry of the Coulomb problem allows for its exact solution by purely algebraic means. We know 7 constants of motion, energy $H$, angular momentum $\vec{L} = \vec{r} \times \vec{p}$, and the Runge-Lenz vector

$$\vec{F} = \frac{1}{2}(\vec{p} \times \vec{L} - \vec{L} \times \vec{p}) + m\alpha \frac{\vec{r}}{|\vec{r}|}. \quad (324)$$

As $[\vec{p}, \vec{L}] \neq 0$, the explicitly hermitian form of the $\times$-product appears here. We have emphasized here how mass $m$ and charge $\alpha = qZ$ (positive $\alpha$ for repulsive potentials) enter the constants. The constants are not algebraically independent but there are relations between them. This is to be expected from the corresponding classical system: there, the constants are functions in phase space and there cannot be more independent constants then the 6 dimensions of the phase space.

In fact, the 7 constants of motion generate an algebra that is isomorphic to the algebra of two sets of angular momenta in the case of the bound states.

Problem 7.31: Symmetries of the H-atom

(a) The constants of motion fulfill the following commutation relations

$$[H, L_n] = 0, \quad [L_n, F_l] = i\epsilon_{nl} F_s$$
$$[H, F_n] = 0, \quad [F_n, F_l] = -2mH i\epsilon_{nl} L_s$$
$$\vec{L} \cdot \vec{F} = \vec{F} \cdot \vec{L} = 0$$
$$\vec{F}^2 = 2mH(\vec{L}^2 + 1) + m\alpha^2$$

Verify this by explicit calculation.

(b) Let $P = \sum_{nlm} |nlm\rangle \langle nlm|$ be the projector onto the bound state spectrum. Then

$$A_n := L_n + F_n \sqrt{-2mH}/2, \quad B_n := L_n - F_n \sqrt{-2mH}/2 \quad (325)$$

are well-defined and fulfill the algebra of two independent angular momentum operators:

$$[A_i, A_j] = i\epsilon_{ijk} A_k, \quad [B_i, B_j] = i\epsilon_{ijk} B_k, \quad [A_i, B_j] = 0. \quad (326)$$
Verify this.

(c) Convince yourself of

\[ \vec{A}^2 = \vec{B}^2 = -\left(\frac{1}{4} + \frac{m\alpha^2}{8\bar{H}}\right) P \]  

(327)

(d) Remember that for any vector of operators \( \vec{X} \) obeying an angular momentum algebra one has the spectra

\[ \sigma(X_m) = \frac{1}{2}\{ \ldots - 2, -1, 0, 1, 2 \ldots \} \]

\[ \sigma(\vec{X}^2) = \frac{1}{4}\{0, 1(1 + 2), 2(2 + 2), 3(3 + 2), \ldots \} \]

and use (327) to derive the Balmer formula.

Note that the \( \vec{A}, \vec{B} \) form the Lie-algebra of the \( SO(4) \) symmetry group, i.e. rotations in \( \mathbb{R}^4 \).

7.5 Exact Coulomb scattering

In the limit of large times \( t \to \pm \infty \), we can in all of these constants of motion replace the operators \( \vec{p} \) and \( \vec{r}/|\vec{r}| \) by their asymptotic values, if we restrict ourselves to the continuous spectrum by using the projector \( Q = (1 - P) \). But as they are constants, the limit value is equal to the value at any time, i.e.

\[ QHQ = \frac{1}{2}\vec{p}_\pm^2 \]

\[ Q\vec{F}Q = \frac{1}{2}(\vec{p}_\pm \times \vec{L} - \vec{L} \times \vec{p}_\pm) \pm m\alpha \frac{\vec{p}_\pm}{|\vec{p}_\pm|}. \]

\[ = \frac{1}{2}[\vec{p}_\pm, \vec{L}^2] \pm m\alpha \frac{\vec{p}_\pm}{|\vec{p}_\pm|} \]

Note: we have exactly the same algebra in classical mechanics, replacing commutators with Poisson brackets.

From these equations, one can derive a relations between \( \vec{p}_+ \) and \( \vec{p}_- \)
(show by evaluating $\vec{F} \times \vec{L}$):

\[
\vec{p}_+ = \vec{p}_- \left( L_2^2 + i\eta - \eta^2 \right) + (\vec{p}_- \times \vec{L} - \vec{L} \times \vec{p}_-) \frac{\eta}{L_2^2 - i\eta + \eta^2}
\]  
\[
= \vec{p}_- \frac{L_2^2(1 + i\eta) + i\eta - \eta^2}{L_2^2 - i\eta + \eta^2} - i\eta L_2^2 \vec{p}_- \frac{1}{L_2^2 - i\eta + \eta^2}
\]

\[
\eta(H) := \frac{Q m\alpha}{\sqrt{2mH}}
\]

7.5.1 Scattering transformation

\[
S = \frac{\Gamma\left(\frac{1}{2} - \sqrt{L_2^2 + \frac{1}{4} + i\eta(H)}\right)}{\Gamma\left(\frac{1}{2} - \sqrt{L_2^2 + \frac{1}{4} - i\eta(H)}\right)}
\]

with the property

\[
\vec{p}_+ = S^{-1} \vec{p}_- S.
\]

This has the form $A^\dagger A^{-1}$ with $A$ being “normal” ($[A, A^\dagger] = 0$, it is therefore unitary.

This can be shown as follows: In a angular expansion and spectral representation w.r.t. $E = 2k^2$ it is

\[
S|l, m\rangle \otimes |\phi(k)\rangle = e^{2i\delta_{l}(k)}|l, m\rangle \otimes |\phi(k)\rangle
\]

The phase can be determined by computing matrix elements for the $z$-components of $\vec{p}_\pm$: this conserves $m$, but changes angular momentum by one:

\[
\langle l + 1, m | (\vec{p}_+) | l, m \rangle = \langle l + 1, m | (\vec{p}_-) | l, m \rangle \frac{l(l+1)(1+i\eta) + i\eta - \eta^2}{l(l+1) - i\eta + \eta^2} - i\eta(l+2)(\vec{p}_-) \frac{1}{l(l+1) - i\eta + \eta^2}\]

\[
\langle l + 1, m | (\vec{p}_-) | l, m \rangle \frac{l(l+1) - i\eta(2l+1) - \eta^2}{l(l+1) - i\eta + \eta^2} = \langle l + 1, m | (\vec{p}_-) | l, m \rangle \frac{(l+1-i\eta)(l-i\eta)}{(l+1+i\eta)(l-i\eta)}
\]

from which one obtains

\[
\frac{\langle l + 1, m | (\vec{p}_+) | l, m \rangle}{\langle l + 1, m | (\vec{p}_-) | l, m \rangle} = \frac{l + 1 - i\eta}{l + 1 + i\eta} = e^{2i(\delta_l - \delta_{l+1})}
\]

The scattering phase is fixed only up to a given overall phases and we fix it by

\[
e^{2i\delta_0(k)} = \frac{\Gamma(1 + i\eta(k))}{\Gamma(1 - i\eta(k))}.
\]
By the property of the $z \Gamma(z) = \Gamma(z + 1)$ we obtain the result for $l > 0$.

### 7.5.2 Scattering cross section

Although we have not run the full program of scattering theory, we can still compute the exact cross section using the $S$-operator. Note that $S$ is in the Heisenberg picture, i.e. it maps within $\mathcal{H}_{ac}(H)$, not within $\mathcal{H}_{ac}(H_0)$. Therefore, we cannot consider an arbitrary $\phi \in \mathcal{H} = \mathcal{H}_{ac}(H_0) \neq \mathcal{H}_{ac}(H)$ and apply $S$.

However, we can simply identify $S$ with some $S_{00}$ (in the interaction picture) of a scattering problem that has the same mapping of momenta which is all we care about usually. The difference between $S$ and $S_{00}$ could be that $S$ maps a given wave-packet $\phi \in \mathcal{H}_{ac}(H)$ to a larger distance at the outgoing side than $S_{00}$, but into the same direction, which is the only thing that matters, as energy is guaranteed to be conserved.

Considering this fictitious comparison system, we can use the usual apparatus of scattering theory to determine the cross sections. In particular we can use the relation between scattering phases and scattering amplitude:

$$f(k, \vec{n}, \vec{n}') = \sum_{l=0}^{\infty} \frac{2l + 1}{2ik} P_l(\cos \theta) \left[ \frac{\Gamma(1 + l + i\eta)}{\Gamma(1 + l - i\eta)} \right]$$

This actually evaluates by several non-elementary manipulations to

$$f(k, \vec{n}, \vec{n}') = \frac{i\eta}{2k} \left( \frac{4}{|\vec{n} - \vec{n}'|} \right)^{1+i\eta} \frac{\Gamma(1 + i\eta)}{\Gamma(1 - i\eta)} - \frac{1}{2ik} \delta^{(2)}(\vec{n} - \vec{n}')$$

Note that all complex contributions here are just phases and, avoiding $\vec{n} = \vec{n}'$, we recover the classical cross section

$$\sigma(k, \vec{n}, \vec{n}') = |f(k, \vec{n}, \vec{n}')|^2 = \frac{\alpha^2}{16E \sin^4(\theta/2)}.$$  

### 7.5.3 Coulomb functions

For completeness we mention the Coulomb functions that solve the eigen-value equation [Abramowitz 1954]

$$\frac{d^2}{d\rho^2} W + \left[ 1 - \frac{2\eta}{\rho} - \frac{l(l + 1)}{\rho^2} \right] W = 0.$$  

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Here, all parameter- and energy dependence has been absorbed into $\eta$, which is exactly the $\eta$ we had defined previously:

$$\eta(E) = \frac{meZ}{\sqrt{2mE}} = \frac{meZ}{k}.$$  \hfill (340)

Inserting into (339) and setting $\rho = kr$ and multiplying by $-k^2/2$, we recover the familiar equation for hydrogen-like problems:

$$\left[ -\frac{1}{2} \frac{d^2}{dr^2} + \frac{meZ}{r} - \frac{l(l+1)}{2r^2} - \frac{k^2}{2} \right] W = 0.$$  \hfill (341)

There are regular $F_l(\eta, \rho)$ and irregular $G_l(\eta, \rho)$ solutions with the asymptotics

$$G_l(\eta, \rho) + iF_l(\eta, \rho) \sim \exp\left[ i(\rho - \eta \log(2\rho) - l\pi/2 + \sigma_l) \right]$$  \hfill (342)

where scattering phases are $\sigma_l = \arg \Gamma(l+1+i\eta)$. As to be expected, this is not asymptotically free motion, rather there is a logarithmic phase slip.

As is known, these can be expressed in terms of confluent hypergeometric functions, in various forms and a range of asymptotic expressions are known. (See, e.g., the “Digital Library of Mathematical Functions”, hosted at NIST. Also, computer codes are provided, e.g. in the Gnu Scientific Library to evaluate them. Unfortunately, handling these functions is far more difficult than handling plane waves with the related Fourier transforms.

### 7.6 Coulomb plus short range potentials

A large class of scattering problems can be described by potentials

$$V(r) = V_s + \frac{q}{r}.$$  \hfill (343)

For these problems we expect scattering theory to exist for the comparison Hamiltonian

$$H_q = -\frac{1}{2} \Delta + \frac{q}{r}.$$  \hfill (344)