10 Scattering Matrix

When we computed some simple scattering processes we did not really know what we were doing. At leading order this did not matter, but at higher orders complications arise. Let us therefore discuss the asymptotic particle states and their scattering matrix in more detail.

10.1 Asymptotic States

First we need to understand asymptotic particle states in the interacting theory

$$|p_1, p_2, \ldots\rangle. \tag{10.1}$$

In particular, we need to understand how to include them in calculations by expressing them in terms of the interacting field $\phi(x)$.

Asymptotic particles behave like free particles at least in the absence of other nearby asymptotic particles. For free fields we have seen how to encode the particle modes into two-point correlators, commutators and propagators. Let us therefore investigate these characteristic functions in the interacting model.

Two-Point Correlator. Consider first the correlator of two interacting fields

$$\mathit{\Delta}_+(x-y) := \langle 0|\phi(x)\phi(y)|0\rangle. \tag{10.2}$$

Due to Poincaré symmetry, it must take the form

$$\mathit{\Delta}_+(x) = \int \frac{d^4p}{(2\pi)^4}\, e^{-ip\cdot x}\, \theta(p_0)\rho(-p^2). \tag{10.3}$$

The factor $\theta(p_0)$ ensures that all excitations of the ground state $|0\rangle$ have positive energy. The function $\rho(s)$ parametrises our ignorance. We do not want tachyonic excitations, hence the function should be supported on positive values of $s = m^2$. We now insert a delta function to express the correlator in terms of the free two-point correlator $\mathit{\Delta}_+(s; x, y)$ with mass $\sqrt{s}$ (Källén, Lehmann)

$$\begin{aligned}\mathit{\Delta}_+(x) &= \int_0^\infty \frac{ds}{2\pi}\, \rho(s) \int \frac{d^4p}{(2\pi)^4}\, e^{-ip\cdot x}\, \theta(p_0) 2\pi\delta(p^2+s)\\ &= \int_0^\infty \frac{ds}{2\pi}\, \rho(s)\mathit{\Delta}_+(s; x). \end{aligned}\tag{10.4}$$

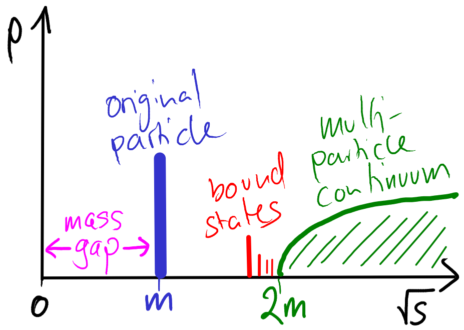
This identifies $\rho(s)$ as the spectral function for the field $\phi(x)$: It tells us by what amount particle modes of mass $\sqrt{s}$ will be excited by the field $\phi(x)$.[1]

[1]The spectral function describes the spectrum of quantum states only to some extent. However, not all states may be excited by the action of a single $\phi(x)$. In particular, in a model with several fields, each field can excite only a subset of particles or states (e.g. the appropriate charges have to match).

Spectral Function. For a free field of mass m_0 we clearly have

$$\rho_0(s) = 2\pi\delta(s - m_0^2). \tag{10.5}$$

For weakly interacting fields, we should obtain a similar expression. In typical situations we expect the spectral function to have the following shape



(10.6)

The sharp isolated peak represents a single particle excitation with mass m. Now the field $\phi(x)$ may also excite multi-particle modes (with the same quantum numbers). Multi-particle modes in the free theory would have energy $e \geq 2m$. In the spectral function they form a continuum since the momenta of the individual particles can sum up to arbitrary energies in the frame at rest. In the presence of interactions, bound states may form whose rest energies are somewhat below $e = 2m$. Whenever these bound states are stable they will also be represented by sharp peaks.

We observe that our spectral function has at least two mass gaps: One separates the vacuum from the lowest excitation; the other separates this latter from bound states and the multi-particle continuum. The isolated modes are called asymptotic particles. This is the type of particle which we would like to collide. The assumption of a mass gap is crucial in this definition.

For weak interactions, we expect that the free particle mode approximates the asymptotic particle well.[2] The interactions may shift the mass $m_0 \to m$ slightly; they may also change the strength with which this mode is excited by the field $\phi(x)$. Therefore the weakly interacting spectral function takes the form

$$\rho(s) = 2\pi Z\delta(s - m^2) + \text{bound states} + \text{continuum}. \tag{10.7}$$

The factor Z is called field strength or wave function renormalisation.

Asymptotic Particles. Based on the above discussion we can expand the field $\phi(x)$ as

$$\phi(x) = \underbrace{\sqrt{Z}\phi_{\text{as}}(x)}_{a^\dagger + a} + \underbrace{\text{bound states} + \text{continuum}}_{(a^\dagger)^n + a^n} + \underbrace{\text{operators}}_{(a^\dagger)^m a^n}. \tag{10.8}$$

[2] For reasonably strong interactions, bound states may approach the single particle states and even acquire lower energies. This case shows that the notion of fundamental particles is not evident in general QFT, but it belongs to weakly interacting models. In fact, some models may have alternative formulations where the fundamental degrees of freedom are some bound states of the original formulation.

Here $\phi_{\text{as}}(x)$ is a canonically normalised free field of mass m expressed by means of creation and annihilation operators $a^\dagger, a$

$$\phi_{\text{as}}(x) = \int \frac{d^3\vec{p}}{(2\pi)^3\, 2e(\vec{p})} \bigl(e^{-ip\cdot x} a(\vec{p}) + e^{ip\cdot x} a^\dagger(\vec{p})\bigr). \tag{10.9}$$

The other terms in the field $\phi(x)$ are multiple creation and/or annihilation operators.

Single particle asymptotic states are created simply by $a^\dagger(\vec{p})$ from the vacuum. The Hamiltonian H_{as} for the free asymptotic field reads

$$H_{\text{as}} = \int \frac{d^3\vec{p}}{(2\pi)^3\, 2e(\vec{p})}\, e(\vec{p}) a^\dagger(\vec{p}) a(\vec{p}). \tag{10.10}$$

The characteristic property of H_{as} is that it reproduces exactly the time evolution of the vacuum and single-particle states

$$H_{\text{as}}|0\rangle = 0 = H|0\rangle, \quad H_{\text{as}} a^\dagger(\vec{p})|0\rangle = e(\vec{p}) a^\dagger(\vec{p})|0\rangle = H a^\dagger(\vec{p})|0\rangle. \tag{10.11}$$

We shall use the free creation and annihilation operators as some convenient basis to expand our interacting fields. The omitted terms in the field $\phi(x)$ are some higher-order polynomials in the operators $a^\dagger, a$ which create and annihilate bound state particles and states from the multi-particle continuum.

Commutator and Normalisation. The other characteristic functions now follow from our expression for the correlator. As before these can be expressed as convolutions of the same spectral function $\rho(s)$ with their free counterparts.

The expectation value of the unequal time commutator

$$\mathit{\Delta}(x-y) := \langle 0|[\phi(\vec{x}), \phi(\vec{y})]|0\rangle \tag{10.12}$$

therefore reads

$$\mathit{\Delta}(x) = \int_0^\infty \frac{ds}{2\pi}\, \rho(s) \mathit{\Delta}(s; x). \tag{10.13}$$

We know that for a normalised free field the equal time commutation relations imply $-\dot{\mathit{\Delta}}(s; 0, \vec{x}) = i\delta^3(\vec{x})$. Hence

$$\langle 0|[\phi(\vec{x}), \dot{\phi}(\vec{y})]|0\rangle = -\dot{\mathit{\Delta}}(0, \vec{x}-\vec{y}) = i\delta^3(\vec{x}) \int_0^\infty \frac{ds}{2\pi}\, \rho(s). \tag{10.14}$$

Assuming that the field $\phi(x)$ is canonically normalised,[3] we have the constraint

$$\int_0^\infty \frac{ds}{2\pi}\, \rho(s) = 1. \tag{10.15}$$

When using the above expansion of the real field $\phi(x)$ in terms of creation and annihilation operators, it also follows that the function $\rho(s)$ must be positive. Hence the coefficient Z for the asymptotic modes should be between 0 and 1.

[3] This is evident at least if the interaction terms do not contain derivatives.

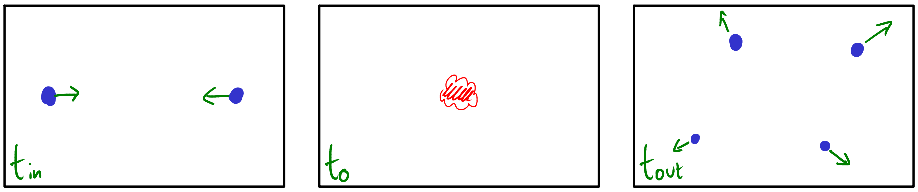
10.2 S-Matrix

For the scattering setup we define two asymptotic regions of spacetime, one in the distance past $t_{\text{in}} \to -\infty$ and one in the distant future $t_{\text{out}} \to +\infty$.

Asymptotic Regions. On the initial time slice we create wave packets which are well separated in position space and narrowly peaked in momentum space. We let these quantum mechanical wave packets evolve in time. At some instance the wave packets collide. Then the state is evolved further until all outgoing wave packets are sufficiently well separated

$$|\text{f}\rangle = \exp\bigl(-iH(t_{\text{out}} - t_{\text{in}})\bigr)|\text{i}\rangle. \tag{10.16}$$

Now the initial and final states are in the Schrödinger picture and they evolve even at asymptotic times. It is hard to compare them to see what the effect of scattering is.[4]



(10.17)

At asymptotic times the wave packets are assumed to be sufficiently well separated such that they effectively do not interact. Therefore we can use the asymptotic Hamiltonian of the asymptotic field ϕ_{as} [5]

$$H_{\text{as}} = \int \frac{d^3\vec p}{(2\pi)^3\, 2e(\vec p)}\, e(\vec p) a^\dagger(\vec p) a(\vec p). \tag{10.18}$$

to shift the two time slices onto a common one conventionally positioned at $t = 0$

$$|\text{out}\rangle = \exp\bigl(iH_{\text{as}} t_{\text{out}}\bigr)|\text{f}\rangle, \qquad |\text{i}\rangle = \exp\bigl(-iH_{\text{as}} t_{\text{in}}\bigr)|\text{in}\rangle. \tag{10.19}$$

The relationship between the in and out states is the following

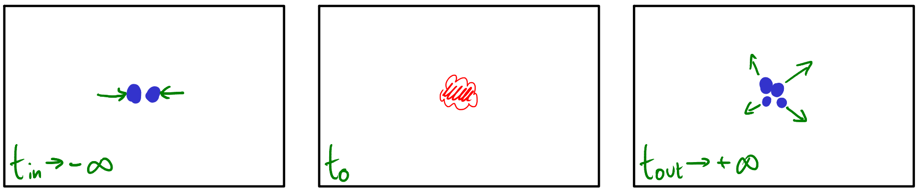
$$\begin{aligned} |\text{out}\rangle &= \exp\bigl(iH_{\text{as}} t_{\text{out}}\bigr) \exp\bigl(-iH(t_{\text{out}} - t_{\text{in}})\bigr) \exp\bigl(-iH_{\text{as}} t_{\text{in}}\bigr)|\text{in}\rangle \\ &=: U_{\text{as}}(t_{\text{out}}, t_{\text{in}})|\text{in}\rangle. \end{aligned} \tag{10.20}$$

The in and out states $|\text{in}\rangle$ and $|\text{out}\rangle$ are both defined at time $t = 0$. Consequently, they are elements of the same Hilbert space and can be compared directly. The

[4]The latter figure is somewhat misleading in a quantum mechanical setting. It shows only one out of many potential final states.

[5]This asymptotic Hamiltonian is a specialisation of the free Hamiltonian H_0 used previously in the interaction picture. The free Hamiltonian was merely required to agree with the full Hamiltonian at leading order. The asymptotic Hamiltonian furthermore has to agree with the full Hamiltonian exactly when action on the vacuum or one-particle states.

operator U_{as} is the time evolution operator for the interaction picture based on the asymptotic Hamiltonian H_{as} and the reference time slice at $t = 0$.



(10.21)

S-Matrix Definition. As interactions have become negligible at asymptotic times, the in and out states are almost independent of t_{in} and t_{out}. It therefore makes sense to take the limit $t_{\mathrm{in,out}} \to \mp\infty$. The limit of the time evolution operator for infinite times is called the S-matrix

$$\begin{aligned} S &= \lim_{t_{\mathrm{in,out}} \to \mp\infty} \exp\bigl(iH_{\mathrm{as}} t_{\mathrm{out}}\bigr) \exp\bigl(iH(t_{\mathrm{in}} - t_{\mathrm{out}})\bigr) \exp\bigl(-iH_{\mathrm{as}} t_{\mathrm{in}}\bigr). \\ &= \lim_{t_{\mathrm{in,out}} \to \mp\infty} U(t_{\mathrm{out}}, t_{\mathrm{in}}) = U(+\infty, -\infty). \end{aligned} \tag{10.22}$$

It transforms in states to out states

$$|\mathrm{out}\rangle = S|\mathrm{in}\rangle. \tag{10.23}$$

Note that the in and out Hilbert spaces are isomorphic.[6] This allows us to compare states between the two. To compute matrix elements of the S-matrix, prepare definite in and out states[7] using the creation and annihilation operators $a^\dagger, a$

$$\begin{aligned} |\mathrm{in}\rangle &= |p_1, \ldots, p_m\rangle := a^\dagger(\vec{p}_1) \ldots a^\dagger(\vec{p}_m)|0\rangle, \\ \langle\mathrm{out}| &= \langle q_1, \ldots, q_n| := \langle 0|a(\vec{q}_1) \ldots a(\vec{q}_n). \end{aligned} \tag{10.24}$$

Conventionally, scattering amplitudes M are defined as the matrix elements of $S - 1$ with the overall momentum-conserving delta function stripped off

$$\langle\mathrm{out}|(S-1)|\mathrm{in}\rangle = (2\pi)^4 \delta^4(P_{\mathrm{in}} - P_{\mathrm{out}}) iM(p_1, \ldots p_m; q_1, \ldots, q_n). \tag{10.25}$$

The combination $S - 1$ is particularly useful for $2 \to n$ scattering processes: It removes all direct connections between the in and out states as well as all other disconnected contributions.[8]

Properties of the S-Matrix. The S-matrix has a number of useful properties, let us list a few relevant ones.

First of all, the S-matrix is trivial for the ground state and for single-particle states

$$S|0\rangle = |0\rangle, \qquad S|\vec{p}\rangle = |\vec{p}\rangle. \tag{10.26}$$

[6]It is natural to assume that outgoing particles of some scattering process can be used as ingoing particles of another scattering process. Therefore the in and out spaces must be isomorphic.

[7]These in and out states are not to be related by $|\mathrm{out}\rangle = S|\mathrm{in}\rangle$.

[8]When one of the ingoing particles does not participate in the scattering, the S-matrix must act trivially on the other. For general $m \to n$ scattering, the matrix elements indeed contain direct connections and disconnected contributions.

This follows from the definition of the asymptotic Hamiltonian to strictly emulate the action of the interacting Hamiltonian on these states.

The S-matrix is a unitary operator

$$S^\dagger = S^{-1}. \tag{10.27}$$

This property follows from the definition. It reflects the fact that probabilities are conserved across scattering processes.

The S-matrix is also Poincaré invariant

$$U(\omega, a) S U(\omega, a)^{-1} = S. \tag{10.28}$$

10.3 Time-Ordered Correlators

When we expressed the time-evolution operator in the interaction picture, we realised that time-ordered correlation functions $\langle \phi(x_1) \ldots \phi(x_n) \rangle$ are very natural objects. The S-matrix is defined as the time evolution operator for the interaction picture in terms of asymptotic states. Lehmann, Symanzik and Zimmermann derived a relationship between the S-matrix elements and time-ordered expectation values.

Asymptotic States. First we need to understand how to represent particle creation and annihilation operators $a^\dagger, a$ in terms of the field $\phi(x)$. Above we have expanded the field $\phi(x)$ as

$$\phi(x) = \sqrt{Z} \int \frac{d^3\vec p}{(2\pi)^3\, 2e(\vec p)} \bigl(e^{-ip\cdot x} a(\vec p) + e^{ip\cdot x} a^\dagger(\vec p)\bigr) + \ldots. \tag{10.29}$$

The omitted terms represent the contributions from multi-particle states and operators which annihilate the vacuum.

Previously we were able to isolate $a^\dagger(\vec p)$ from a time slice of the free field $\phi_0(x)$ as

$$a^\dagger(\vec p) = \int d^3\vec x\, e^{-ip\cdot x} \bigl(e(\vec p)\phi_0(x) - i\dot\phi_0(x)\bigr). \tag{10.30}$$

This was easy because there are only two modes with $e = \pm e(\vec p)$ in the free field ϕ_0. The linear combination of ϕ and $\dot\phi$ selects the correct one.

The interacting field, however, in general carries many other modes whose precise nature we do not understand a priori. To select the modes corresponding to $a^\dagger$ and a we need to drive the field $\phi(x)$ for a sufficiently long time with a frequency that is in resonance with the relevant modes. Let us sketch the construction for a single oscillator $f(t) = ce^{i\omega t}$ with resonance frequency ω

$$F(e) = \int_{t_1}^{t_2} dt\, e^{-iet} f(t) = \frac{ic}{e-\omega}\bigl(e^{-i(e-\omega)t_2} - e^{-i(e-\omega)t_1}\bigr) \tag{10.31}$$

The longer the time, the stronger will be the amplitude at $e = \omega$. At infinite time the function $F(e)$ develops a pole at e, so we set $t_1 = -\infty$

$$F(e) = \int_{-\infty}^{t_2} dt\, e^{-iet} f(t) = \frac{ice^{-i(e-\omega)t_2}}{e-\omega} = \frac{ic}{e-\omega} + \text{finite}. \tag{10.32}$$

Here we have discarded the term that keeps oscillating at asymptotic times.[9] What remains is an isolated pole at $e = \omega$ whose residue is proportional to the amplitude c. The residue is in fact independent of the time t_2 where the driving stops.

Applied to the field $\phi(x)$ we find

$$\int_{-\infty}^{t_2} dt \int d^3\vec{x}\, e^{-ip\cdot x}\phi(x) \tag{10.33}$$

$$= \frac{i\sqrt{Z}}{p^2+m^2}\big(\theta(-e)a_{\text{in}}(-\vec{p}) - \theta(e)a^\dagger_{\text{in}}(\vec{p})\big) + \ldots. \tag{10.34}$$

What remains are isolated poles at $e = \pm e(\vec{p})$ whose residues are creation and annihilation operators for ingoing asymptotic particles. The remaining terms are either finite or irrelevant when creating well-separated wave packets. We decided to shift the ingoing Fock space back to the time $t = 0$ using the free asymptotic Hamiltonian. Therefore we conjugate the creation and annihilation operators by the appropriate time evolution operator

$$a_{\text{in}}(\vec{p}) = U(0,-\infty)a(\vec{p})U(-\infty,0). \tag{10.35}$$

We note:

- The residues of the pole $1/(p^2+m^2)$ isolate the creation and annihilation operators.[10]
- The residues at positive and negative energies correspond to creation and annihilation operators, respectively.
- The residues do not depend on the final time t_2.
- Bound state particles correspond to similar poles at different energies.

A similar expression with opposite sign is obtained for driving the field into the distant future

$$\int_{t_1}^{\infty} dt \int d^3\vec{x}\, e^{-ip\cdot x}\phi(x) \tag{10.36}$$

$$= -\frac{i\sqrt{Z}}{p^2+m^2}\big(\theta(-e)a_{\text{out}}(-\vec{p}) - \theta(e)a^\dagger_{\text{out}}(\vec{p})\big) + \ldots. \tag{10.37}$$

Here we identify

$$a_{\text{out}}(\vec{p}) = U(0,+\infty)a(\vec{p})U(+\infty,0). \tag{10.38}$$

[9] As usual, one could formally dampen this term by introducing some small imaginary part. This may be an approximation, but even in practice, one can *never* isolate a resonance perfectly.

[10] The can be further operators consisting of several creation and annihilation operators.

LSZ Reduction. We want to express the elements of the S-matrix in terms of time-ordered correlation functions in momentum space. Let us start with the time-ordered expectation value

$$F_{m,n}(p,q) = \int \prod_{k=1}^{m} \bigl(d^4x_k\, e^{-ip_k\cdot x_k}\bigr) \prod_{k=1}^{n} \bigl(d^4y_k\, e^{iq_k\cdot y_k}\bigr) \\ \langle 0|\mathrm{T}\bigl(\phi(x_1)\ldots\phi(x_n)\phi(y_1)\ldots\phi(y_m)\bigr)|0\rangle. \tag{10.39}$$

Consider just the integral of the quantum operator over one of the x_k

$$X = \int d^4x\, e^{-ip\cdot x}\mathrm{T}\bigl(\phi(x)Y\bigr). \tag{10.40}$$

Now split up the time integral into three regions at the times t_{min} and t_{max} representing the minimal and maximal times within the operator Y

$$\begin{aligned} X = {}& \int_{-\infty}^{t_{\text{min}}} dt \int d^3\vec{x}\, e^{-ip\cdot x}\mathrm{T}(Y)\phi(x) \\ &+ \int_{t_{\text{min}}}^{t_{\text{max}}} dt \int d^3\vec{x}\, e^{-ip\cdot x}\mathrm{T}\bigl(\phi(x)Y\bigr) \\ &+ \int_{t_{\text{max}}}^{+\infty} dt \int d^3\vec{x}\, e^{-ip\cdot x}\phi(x)\mathrm{T}(Y). \end{aligned} \tag{10.41}$$

According to the results of the above consideration of resonances, the two integrals extending to $t = \pm\infty$ produce a pole when the momentum is on shell, $p^2 = -m^2$. Conversely, the middle integral is finite and therefore does not produce a pole. We can express the residue of the pole using creation operators of in and out particles

$$X \simeq \frac{-i\sqrt{Z}}{p^2+m^2}\Bigl(\mathrm{T}(Y)a^\dagger_{\text{in}}(\vec{p}) - a^\dagger_{\text{out}}(\vec{p})\mathrm{T}(Y)\Bigr), \tag{10.42}$$

where we discard finite contributions at $p^2 = -m^2$. Performing this step for all ingoing particles yields

$$\begin{aligned} F_{m,n} \simeq {}& \prod_{k=1}^{m}\left(\frac{-i\sqrt{Z}}{p_k^2+m^2}\right) \int \prod_{k=1}^{n} \bigl(d^4y_k\, e^{iq_k\cdot y_k}\bigr) \\ & \qquad \langle 0|\mathrm{T}\bigl(\phi(y_1)\ldots\phi(y_m)\bigr)a^\dagger_{\text{in}}(\vec{p}_1)\ldots a^\dagger_{\text{in}}(\vec{p}_m)|0\rangle \\ = {}& \prod_{k=1}^{m}\left(\frac{-i\sqrt{Z}}{p_k^2+m^2}\right) \int \prod_{k=1}^{n} \bigl(d^4y_k\, e^{iq_k\cdot y_k}\bigr) \\ & \qquad \langle 0|\mathrm{T}\bigl(\phi(y_1)\ldots\phi(y_m)\bigr)U(0,-\infty)a^\dagger(\vec{p}_1)\ldots a^\dagger(\vec{p}_m)|0\rangle. \end{aligned} \tag{10.43}$$

Note that all outgoing creation operators $a^\dagger_{\text{out}}$ directly annihilate the vacuum $\langle 0|$.

Now we perform equivalent steps for the outgoing particles. We use a similar relation as above dressed by factors of $U(+\infty,0)$ and $U(0,-\infty)$

$$X = \int d^4y\, e^{iq\cdot y} U(+\infty,0)\mathrm{T}\big(\phi(y)Y\big)U(0,-\infty). \tag{10.44}$$

$$\simeq \frac{-i\sqrt{Z}}{q^2+m^2}\Big(U(+\infty,0)\mathrm{T}(Y)a_{\mathrm{in}}(\vec{q})U(0,-\infty) \tag{10.45}$$

$$- U(+\infty,0)a_{\mathrm{out}}(\vec{q})\mathrm{T}(Y)U(0,-\infty)\Big), \tag{10.46}$$

$$\simeq \frac{-i\sqrt{Z}}{q^2+m^2}\,[U(+\infty,0)\mathrm{T}(Y)U(0,-\infty), a(\vec{q})]. \tag{10.47}$$

For each particle this yields one commutator of the remaining fields $U(+\infty,0)\mathrm{T}(Y)U(0,-\infty)$ with an annihilation operator. After performing this step for all the outgoing particles, we are left with the S-matrix

$$U(+\infty,0)\mathrm{T}(1)U(0,-\infty) = S. \tag{10.48}$$

Altogether we find that the residue of $F_{m,n}$ is given by an element of the S-matrix

$$F_{m,n} \simeq \prod_{k=1}^{m}\left(\frac{-i\sqrt{Z}}{p_k^2+m^2}\right)\prod_{k=1}^{n}\left(\frac{-i\sqrt{Z}}{q_k^2+m^2}\right) \langle 0|[a(\vec{q}_1),\ldots[a(\vec{q}_n),S]\ldots]a^\dagger(\vec{p}_1)\ldots a^\dagger(\vec{p}_m)|0\rangle. \tag{10.49}$$

Here, the commutators make all the $a(\vec{q}_k)$ connect only to the S-matrix. Now there is nothing else left, and therefore also all $a^\dagger(\vec{p}_k)$ must connect to S.

10.4 S-Matrix Reconstruction

We have seen that time-ordered correlation functions have poles when the external fields are on the mass shell of asymptotic particles. The residue of these poles is given by the corresponding element of the scattering matrix.

We can therefore fully reconstruct the S-matrix from time-ordered correlation functions.

Two-Point Correlator. In the construction of the S-matrix, the two-point correlation function takes a special role. First, consider the above residue formula for two legs

$$F_{1,1} \simeq \frac{-i\sqrt{Z}}{p^2+m^2}\,\frac{-i\sqrt{Z}}{q^2+m^2}\,\langle 0|a(\vec{q})(S-1)a^\dagger(\vec{p})|0\rangle. \tag{10.50}$$

Momentum conservation implies $p=q$, hence the residue of a double pole at $p^2=-m^2$ is given by $\langle 0|a(\vec{q})(S-1)a^\dagger(\vec{p})|0\rangle$. However, the S-matrix should act as the identity on single-particle states. We conclude that there is no double pole in $F_{1,1}$ at $p^2=-m^2$. There is no reason to expect a double pole in the first place, therefore the above residue statement is empty for $m=n=1$.

There is nevertheless a single pole at $p^2 = -m^2$ as can be shown using the spectral representation of the time-ordered two-point function

$$F_2(x-y) = \langle \phi(x)\phi(y)\rangle := \langle 0|\mathrm{T}\big(\phi(x)\phi(y)\big)|0\rangle. \tag{10.51}$$

Using the spectral function $\rho(s)$ of the interacting field $\phi(x)$, it can be written in terms of the free Feynman propagator of mass $\sqrt{s}$

$$F_2(x-y) = -i\int_0^\infty \frac{ds}{2\pi}\,\rho(s) G_{\mathrm{F}}(s; x-y). \tag{10.52}$$

Most importantly, its momentum space representation

$$F_2(p) = -i\int_0^\infty \frac{ds}{2\pi}\,\frac{\rho(s)}{p^2+s-i\epsilon} = \frac{-iZ}{p^2+m^2-i\epsilon} + \ldots \tag{10.53}$$

contains the parameters of the asymptotic particle: The function $F_2(p)$ has an isolated pole at the physical mass m, and its residue is the wave function renormalisation factor Z.

Now we can nicely expand F_2 in terms of Feynman diagrams with two external legs and thus determine m and Z.

Amputation. The residue formula for the time-ordered correlation functions can be inverted to a complete expression for the S-matrix

$$S = 1 + \sum_{m,n=2}^{\infty} \int \prod_{k=1}^{n} \frac{d^3\vec q_k\, a^\dagger(\vec q_k)}{(2\pi)^3\, 2e(\vec q)} \prod_{k=1}^{m} \frac{d^3\vec p_k\, a(\vec p_k)}{(2\pi)^3\, 2e(\vec p)} \cdot \left(\frac{F_{m,n}(p,q)}{m!\, n!} \prod_{k=1}^{m} \frac{p_k^2+m^2}{-i\sqrt{Z}} \prod_{k=1}^{n} \frac{q_k^2+m^2}{-i\sqrt{Z}} \right).$$

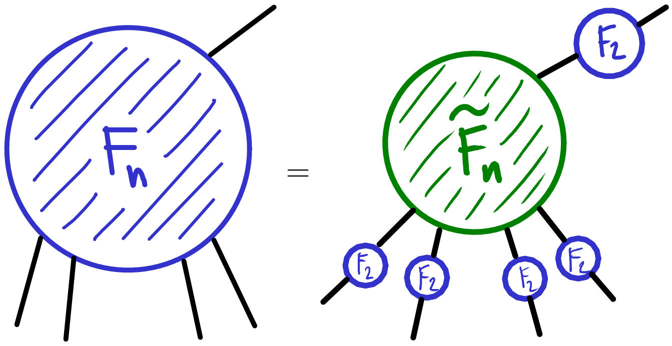
Importantly, the poles and zeros of the latter term must be combined before the momenta are set on shell $p_k^2 = q_k^2 = -m^2$. The construction of this expression ensures that

- the vacuum does not scatter, $S|0\rangle = |0\rangle$,
- single-particle states do not scatter, $S|p\rangle = |p\rangle$,
- for more two or more particles, the residue of $F_{m,n}$ is reproduced according to the above formula.

It is now convenient to replace each factor $(p_k^2 + m^2)$ by the inverse of the corresponding two-point function in the construction of the S-matrix

$$S = 1 + \sum_{m,n=2}^{\infty} \int \prod_{k=1}^{n} \frac{d^3\vec q_k\, a^\dagger(\vec q_k)}{(2\pi)^3\, 2e(\vec q)} \prod_{k=1}^{m} \frac{d^3\vec p_k\, a(\vec p_k)}{(2\pi)^3\, 2e(\vec p)} \cdot \left(\frac{F_{m,n}(p,q)}{m!\, n!} \prod_{k=1}^{m} \frac{\sqrt{Z}}{F_2(p_k)} \prod_{k=1}^{n} \frac{\sqrt{Z}}{F_2(q_k)} \right).$$

This formula has a useful interpretation in terms of Feynman graphs for $F_{m,n}$.



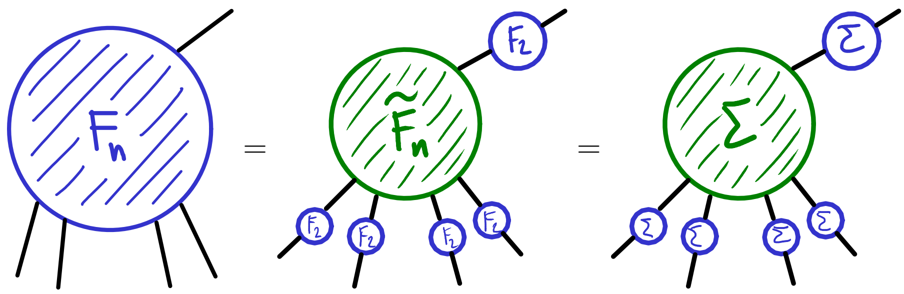
(10.54)

In the second representation we have cut the graph into a smaller $(m+n)$-function and $m+n$ 2-point functions according to the rules:

- Each 2-point function connects an external leg to the $(m+n)$-function at the core.
- Each 2-point function is maximal.
- The Feynman propagator that connects the 2-point function to the core is attributed to the 2-point function.

Essentially one chops each leg of the graph as much as possible. Such a graph is called *amputated*.

Now it is clear that each 2-point fragment of the graph is a Feynman graph for the two-point function F_2. Moreover all these graphs have natural relative weights. The sum of all Feynman graphs contributing to $F_{m,n}$ therefore contains the sum of all graphs contributing to F_2 separately for each leg



(10.55)

What remains is a sum over all amputated Feynman graphs at the core. This expression separates cleanly into factors because all the weights are naturally defined

$$F_{m,n}(p,q) = \tilde{F}_{m,n}(p,q) \prod_{k=1}^{m} F_2(p_k) \prod_{k=1}^{n} F_2(q_k). \tag{10.56}$$

The function $\tilde{F}_{m,n}$ therefore is precisely what is needed for reconstruction of the S-matrix

$$S = 1 + \sum_{m,n=2}^{\infty} \int \prod_{k=1}^{n} \frac{d^3\vec{q}_k\, a^\dagger(\vec{q}_k)}{(2\pi)^3\, 2e(\vec{q})} \prod_{k=1}^{m} \frac{d^3\vec{p}_k\, a(\vec{p}_k)}{(2\pi)^3\, 2e(\vec{p})} \frac{\sqrt{Z}^{m+n}}{m!\, n!} \tilde{F}_{m,n}.$$

In other words, the elements of the S-matrix are determined precisely by the sum of amputated Feynman graphs multiplied by $\sqrt{Z}$ for each external leg.

In General. The general picture is as follows: Poles in the time-ordered two-point function $F_2(p)$ indicate stable asymptotic particle states.[11] [12]

- These may be deformations of the poles in the free theory.
- They may as well be poles corresponding to bound states.
- Also poles for correlators of composite fields are permissible.

The location $p^2 = -m^2$ of the pole defines the mass m of the particle. Time-ordered multi-point correlation functions have poles at these locations. Their overall residue yields the corresponding element of the S-matrix. Some comments:

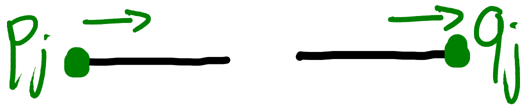
- It is clear that all the external legs of the S-matrix must be exactly on shell.
- Note that in this picture of the S-matrix, crossing symmetry follows from crossing symmetry of time-ordered correlators.
- The S-matrix is completely determined in terms of time-ordered correlation functions. No reference is made to the original formulation of the QFT, e.g. the Lagrangian. This fact will be crucial when we go to higher perturbative orders where Feynman diagrams have internal loops.

Feynman Rules. Let us summarise the Feynman rules for elements of the S-matrix in ϕ^4 theory

$$\langle q_1, \ldots, q_n | S | p_1, \ldots, p_m \rangle. \tag{10.57}$$

The matrix element is given by the sum of all graphs with certain properties. The properties are similar to the properties of Feynman graphs for correlation functions in momentum space, but mainly the external legs are handled differently. Let us state the modified and additional rules:

- The graph has m ingoing and n outgoing external lines labelled by momenta p_k and q_k, respectively.



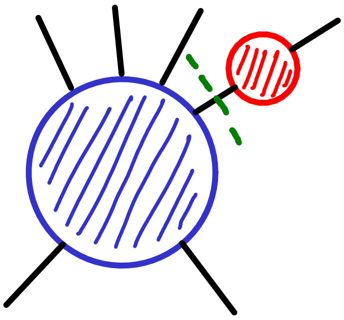
(10.58)

- The external momenta must be on the mass shell, $p_k^2 = q_k^2 = -m^2$, and must have positive energy.
- Cutting the graph at any internal line must not split off a graph with two

[11]When a field has several components, the notion of pole is more subtle in the sense that the residue of a pole is typically a matrix of non-maximal rank, e.g. $p{\cdot}\gamma + m$ for spinor fields. In this case only the vectors which are not projected out correspond to asymptotic particles.

[12]In practice one may not be able to distinguish an exact pole from a very narrow resonance. One might consider such resonances at the same level as stable external particles and allow them as legs of the S-matrix. Such an S-matrix would not rest on rigorous assumptions and therefore not all theorems apply in a strict sense. In this regard, one should remember that in quantum physics one has to make some separation of scales into the microscopic quantum regime and the regime of macroscopic classical objects. Alternatively, resonances can be viewed as asymptotic particles with a complex mass parameter.

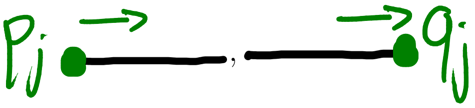
external lines (amputated graph).



$$(10.59)$$

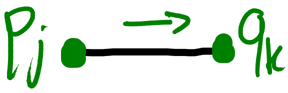
The Feynman rules for evaluating a graph are the same as for correlation functions in momentum space except:

- For each external line write a factor of $\sqrt{Z}$ instead of a Feynman propagator $-i/(p_j^2 + m^2 - i\epsilon)$.



$$\to \sqrt{Z}. \tag{10.60}$$

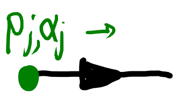
- Any external line which directly connects an ingoing to an outgoing particle contributes a factor of $\langle q_k | p_l \rangle = 2e(\vec{p}_l)(2\pi)^3\delta^3(\vec{p}_l - \vec{q}_k)$. This line simply bypasses the S-matrix.[13]



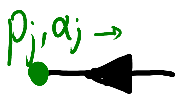
$$\to 2e(\vec{p}_j)\,(2\pi)^3\delta^3(\vec{p}_j - \vec{q}_k). \tag{10.61}$$

For Quantum Electrodynamics the Feynman rules for scattering matrix elements also has to be adjusted w.r.t. the Feynman rules in momentum space, namely:

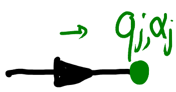
- For each external spinor line, write a factor of $\sqrt{Z_\psi}$ along with $u_\alpha(\vec{q})$, $\bar{u}_\alpha(\vec{p})$, $v_\alpha(\vec{p})$ or $\bar{v}_\alpha(\vec{q})$ depending on whether the particle is in- or outgoing and whether it is an electron or a positron.



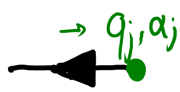
$$\to \sqrt{Z_\psi}\, v_{\alpha_j}(\vec{p}_j),$$



$$\to \sqrt{Z_\psi}\, \bar{u}_{\alpha_j}(\vec{p}_j),$$

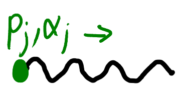


$$\to \sqrt{Z_\psi}\, \bar{v}_{\alpha_j}(\vec{q}_j),$$

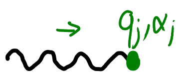


$$\to \sqrt{Z_\psi}\, u_{\alpha_j}(\vec{q}_j) \tag{10.62}$$

- For external photon lines, write a factor of $\sqrt{Z_A}$ along with a normalised transverse polarisation vector $e_\mu(\vec{p})$.



$$\to \sqrt{Z_A}\, \varepsilon_{\alpha_j}(\vec{p}_j),$$



$$\to \sqrt{Z_A}\, \varepsilon^*_{\alpha_j}(\vec{q}_j) \tag{10.63}$$

[13] Such contributions do not directly correspond to the identity within S, i.e. they are present in $S - 1$, but only for at least 3 ingoing particles.

10.5 Unitarity

The S-matrix is a unitary operator

$$S^\dagger = S^{-1}. \tag{10.64}$$

This is an essential feature of any physical QFT. However, when deriving the S-matrix from time-ordered correlators by means of the LSZ reduction, unitarity is not evident at all. Therefore we can use the property to derive some non-trivial relations between elements of the S-matrix.

Optical Theorem. Commonly, an identity operator is removed from the S-matrix as

$$S = 1 + iT. \tag{10.65}$$

This split is useful because for small coupling T is small. Moreover, the identity in S is never seen in LSZ reduction.

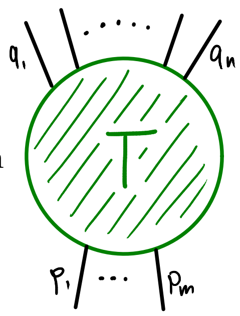
Unitarity $SS^\dagger = 1$ for the operator T is then written as the optical theorem

$$2\,\mathrm{Im}\,T = -iT + iT^\dagger = TT^\dagger = T^\dagger T. \tag{10.66}$$

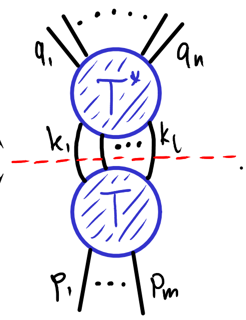
It relates the imaginary part of T to its absolute square. The latter is a quantity we have already encountered: In the form of matrix elements it appears in the scattering cross section. It allows to determine the total cross section of some process in terms of the imaginary part of a matrix element.[14] Alternatively, the imaginary part of T can be obtained as a total cross section,[15] The remaining real part of T can be reconstructed from arguments of complex analyticity.

A graphical representation of the optical theorem is as follows

$$2\,\mathrm{Im}$$



$$= \sum_{l=2}^{\infty} \prod_{j=1}^{l} \int \frac{d^3\vec{k}_j}{(2\pi)^3\, 2e(\vec{k}_j)} \sum_{\text{pol}}$$



$$. \tag{10.67}$$

The optical theorem implies that one has to integrate and sum over all allowed degrees of freedom for these lines which connect T to $T^\dagger$. This is similar as for internal lines within T and $T^\dagger$ with one important distinction: The cut lines originate from contracting two operators a and $a^\dagger$ inside T and $T^\dagger$, respectively,

$$[a(\vec{p}), a^\dagger(\vec{q})] = 2e(\vec{p})\,(2\pi)^3\delta^3(\vec{p}-\vec{q}). \tag{10.68}$$

[14] In this matrix element one would choose the ingoing and outgoing momenta to be the same. Evidently, this requires to split off the momentum-conserving delta function first.

[15] In fact one needs a generalisation of the total cross section where the ingoing particles of T are chosen independently of the outgoing particles of $T^\dagger$.

Therefore the momenta associated to these lines must be on shell, $p^2 = -m^2$, with directed flow of energy p_0 from T towards $T^\dagger$. Conversely, the internal lines are integrated over all off-shell momenta.

Tree Level. It is instructive to discuss the optical theorem at tree level. At first sight one might think that tree-level contributions to T are manifestly real because they are rational functions of the momenta and masses with real coefficients.[16] Although the $i\epsilon$ prescription for Feynman propagators appears negligible, it does have a considerable impact on the imaginary part

$$\frac{1}{p^2 + m^2 - i\epsilon} = \frac{1}{p^2 + m^2} + i\pi\delta(p^2 + m^2). \tag{10.69}$$

Now in the conjugate S-matrix $T^\dagger$ all Feynman propagators are conjugated

$$G_{\mathrm{F}}^*(p) = \frac{1}{p^2 + m^2 + i\epsilon} \neq G_{\mathrm{F}}(p). \tag{10.70}$$

When computing the imaginary part of T one therefore frequently encounters the difference

$$\frac{1}{p^2 + m^2 - i\epsilon} - \frac{1}{p^2 + m^2 + i\epsilon} = 2\pi i\delta(p^2 + m^2). \tag{10.71}$$

This identity replaces the Feynman propagator for an internal line by an on-shell correlator for a cut line connecting T and $T^\dagger$. The restriction to positive energies on the cut is a more subtle issue. It is resolved by the fact that in the sum over all possible cuts each line appears twice, once for every direction of energy flow.

With these remarks one can show that the optical theorem holds at tree level.[17] Here we showed that at tree level T is has an imaginary part concentrated at isolated momentum configurations. However, the optical theorem is most frequently applied at loop level where T is generically complex.

[16] The various prefactors of i for propagators and interaction vertices conspire to cancel out.

[17] Here it is crucial to also take the disconnected contributions to T into account.