6 Interactions and the S-matrix

So far we have been dealing with free, non-interacting quantum field theories for spin-0, spin-$\frac{1}{2}$ and spin-1 particles:

$$\mathcal{L}_0^{\text{sc}} = \frac{1}{2}(\partial\Phi)^2 - \frac{1}{2}m_0^2\,\Phi^2\,, \quad \mathcal{L}_0^{\text{Dirac}} = \bar{\psi}\,(i\partial\!\!\!/ - m_0)\,\psi\,, \quad \mathcal{L}_0^{\text{em}} = -\frac{1}{4}F^2\,. \tag{6.1}$$

We denote the free Lagrangian by $\mathcal{L}_0$ and the mass parameter in the Lagrangian by m_0. We can solve the corresponding equations of motion (the Klein-Gordon, Dirac and Maxwell equations) exactly in terms of superpositions of plane waves. After quantizing such a theory, the Hilbert space is the Fock space of the multiparticle states that are created from the free vacuum $|0\rangle$.

Interactions. What happens when we include interactions? Let's write the interacting Lagrangian as $\mathcal{L} = \mathcal{L}_0 + \mathcal{L}_{\text{int}}$ and the interacting Hamiltonian as $H = H_0 + H_{\text{int}}$. Examples for interactions are:

- Higher-order terms in theories with one type of field, for example the Φ^3 and Φ^4 interactions in a scalar theory: $\mathcal{L}_{\text{int}} = -\frac{g}{3!}\,\Phi^3$ or $\mathcal{L}_{\text{int}} = -\frac{\lambda}{4!}\,\Phi^4$. They describe self-interactions of a scalar particle with respective coupling strengths g and λ.
- Interactions that couple different types of fields, for example the Lagrangian of QED: $\mathcal{L}_{\text{QED}} = \mathcal{L}_0^{\text{Dirac}} + \mathcal{L}_0^{\text{em}} + g\,\bar{\psi}A\!\!\!/\,\psi$.

Later we will see that the possible forms of interactions are tightly constrained by the requirements of gauge invariance and renormalizability.

To keep the discussion generic, let's stick with scalar fields and work out the consequences of their interactions. Unfortunately this complicates matters enormously. Usually we can no longer solve the equations of motion exactly; for example, the Klein-Gordon equation with Φ^3 and Φ^4 interactions becomes

$$(\Box + m_0^2)\,\Phi = -\frac{g}{2}\,\Phi^2 - \frac{\lambda}{3!}\,\Phi^3\,, \tag{6.2}$$

which is non-linear in the fields. Since the field is not free, there is no simple expansion in terms of creation and annihilation operators. At some given time t_0, we could try to expand $\Phi(\boldsymbol{x}, t_0)$ into Fourier modes and formally evolve it with $\Phi(\boldsymbol{x}, t) = e^{iH(t-t_0)}\,\Phi(\boldsymbol{x}, t_0)\,e^{-iH(t-t_0)}$, but H depends on higher powers of Φ which complicates the solution. A state $a_k^\dagger|0\rangle$ can evolve into $a^{\dagger 2}|0\rangle$, $a^\dagger a^2|0\rangle$, $a^{\dagger 3}|0\rangle$ terms etc., which would describe the decay of a one-particle state into two- and three-particle states. Hence, $\Phi(x)$ no longer creates just one-particle states but also **multiparticle states**. Similarly, a fermion operator $\bar{\psi}$ in QED would not only create a single electron but also states that contain an electron plus arbitrarily many photons; A^μ would create states that contain besides a single photon also e^+e^- pairs.

As a consequence, the Hilbert space differs from the free theory: the ground state of the free Hamiltonian H_0 was the free vacuum $|0\rangle$; the ground state of the full Hamiltonian is the interacting vacuum $|\Omega\rangle$. The masses m of the 1-particle momentum eigenstates of H no longer equal the mass parameter m_0 in the Lagrangian. The states interact, and there may be bound states.

The basic quantity of interest is then the **scattering amplitude** or transition amplitude between such multiparticle states. Ideally one would like to find the exact solution of the interacting QFT, compute the exact spectrum and calculate the interactions exactly. Unfortunately such analytic solutions are available only for a few special cases. In general one has to resort to numerical methods (lattice QFT, Dyson-Schwinger equations, functional renormalization-group equations, ...) or simplified models. On the other hand, as long as the couplings are small ($g, \lambda \ll 1$), one can view $\mathcal{L}_{\text{int}}$ as a small perturbation and expand scattering amplitudes in powers of the coupling constant(s). The resulting **perturbation theory** still allows us to perform analytic calculations and it will be our tool of choice in practice. However, before getting there (in Sec. 7), let us first make some general statements that are also valid non-perturbatively.

Källén-Lehmann spectral representation. How can we determine the masses in an interacting quantum field theory? First of all, Lorentz invariance tells us that the commutation relation $[P^\mu, P^\nu] = 0$ must still hold, which implies that the momentum operator commutes with the Hamiltonian and they are simultaneously diagonalizable: $[H, \boldsymbol{P}] = 0$. We label their eigenstates by

$$H\,|\lambda_{\boldsymbol{p}}\rangle = E_p(\lambda)\,|\lambda_{\boldsymbol{p}}\rangle\,, \qquad \boldsymbol{P}\,|\lambda_{\boldsymbol{p}}\rangle = \boldsymbol{p}\,|\lambda_{\boldsymbol{p}}\rangle\,. \tag{6.3}$$

There are now several types of possible Fock states:

- The ground state or vacuum $|\Omega\rangle$, which is invariant under Poincaré transformations. In particular, this means it has zero energy and momentum: $P^\mu|\Omega\rangle = 0$.
- One-particle states $|\boldsymbol{p}\rangle$ with momentum $\boldsymbol{p}$ and energy $E_p = \sqrt{\boldsymbol{p}^2 + m^2}$, where $m \neq m_0$ is no longer the mass parameter in the Lagrangian.
- $N-$particle states that are specified by a center-of-mass momentum $\boldsymbol{p}$, the relative momenta among the particles, and potentially further parameters. For example, the lowest possible energy of a two-particle state in its rest frame ($\boldsymbol{p} = 0$) is $2m$, but since the two particles can have relative momentum, which contributes to their total energy, the state can have *any* energy above $2m$. Therefore, the multiparticle states form a continuum. We write the energy of an $N-$particle state $|\lambda_{\boldsymbol{p}}\rangle$ as $E_p(\lambda) = (\boldsymbol{p}^2 + m_\lambda^2)^{1/2}$, where $m_\lambda \geq 2m$ is the invariant mass of the state (its energy in the rest frame).
- Bound states with mass $< 2m$, which have no analogue in the free theory.

The resulting eigenvalue spectrum of H will generally have the form shown in Fig. 6.1. We can then write the completeness relation for the entire Fock space as

$$\mathbb{1} = |\Omega\rangle\langle\Omega| + \sum_\lambda \int \frac{d^3p}{2E_p(\lambda)}\,|\lambda_{\boldsymbol{p}}\rangle\langle\lambda_{\boldsymbol{p}}|\,. \tag{6.4}$$

The sum over λ is formal and includes integrals over continuous parameters like relative momenta.

Let's have a look at the full **two-point correlation function** $\langle\Omega|\,\mathsf{T}\,\Phi(x)\Phi(y)\,|\Omega\rangle$ for scalar fields (the 'dressed propagator'). We start with $\langle\Omega|\,\Phi(x)\Phi(y)\,|\Omega\rangle$, whose analogue in the free theory is Eq. (2.72). Inserting the completeness relation, we can make the following observations:

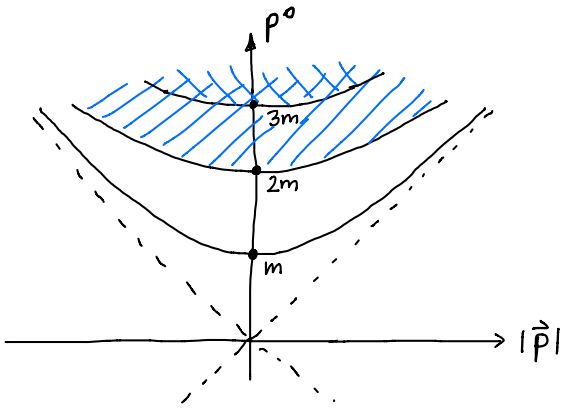

FIGURE 6.1: Eigenvalue spectrum of the Hamiltonian in terms of one-particle states with mass m and multiparticle states with invariant mass $m_\lambda \geq 2m$.

- Remembering Eq. (2.61), we infer that the field behaves under translations as $\Phi(x) = e^{ix\cdot P}\,\Phi(0)\,e^{-ix\cdot P}$. Since the vacuum is translationally invariant, the VEV of a single field $\langle\Omega|\,\Phi(x)\,|\Omega\rangle = \langle\Omega|\,\Phi(0)\,|\Omega\rangle$ must be a constant. We can always redefine the field by subtracting this constant so that the VEV vanishes. (For higher spin fields it vanishes automatically by Lorentz invariance.)

- For the matrix element $\langle\Omega|\,\Phi(x)\,|\lambda_{\boldsymbol{p}}\rangle$ we can also use translation invariance because $\lambda_{\boldsymbol{p}}$ is an eigenstate of P^μ:

$$\langle\Omega|\,\Phi(x)\,|\lambda_{\boldsymbol{p}}\rangle = \langle\Omega|\,e^{ix\cdot P}\,\Phi(0)\,e^{-ix\cdot P}\,|\lambda_{\boldsymbol{p}}\rangle = \langle\Omega|\,\Phi(0)\,|\lambda_{\boldsymbol{p}}\rangle\,e^{-ip\cdot x}\,. \tag{6.5}$$

  If we denote by $U|\lambda_{\boldsymbol{0}}\rangle = |\lambda_{\boldsymbol{p}}\rangle$ a Lorentz boost from the rest frame to the momentum $\boldsymbol{p}$, we can further exploit Lorentz invariance from Eq. (2.65):

$$\langle\Omega|\,\Phi(0)\,|\lambda_{\boldsymbol{p}}\rangle = \langle\Omega|\,U\Phi(0)\,U^{-1}|\lambda_{\boldsymbol{p}}\rangle = \langle\Omega|\,\Phi(0)\,|\lambda_{\boldsymbol{0}}\rangle\,. \tag{6.6}$$

  This quantity measures the overlap of $\langle\Omega|\,\Phi(0)$ with the state $|\lambda_{\boldsymbol{0}}\rangle$. For a one-particle state it is simply a constant, whereas for a general $N-$particle state it still depends on the relative momenta. In the following we will write

$$|\langle\Omega|\,\Phi(0)\,|\lambda_{\boldsymbol{0}}\rangle|^2 =: \frac{Z_{(\lambda)}}{(2\pi)^3}\,. \tag{6.7}$$

  Compare this with the free theory, Eq. (2.35): If $\Phi(x)$ would only create a free particle from the vacuum, then the overlap would be $Z_{(1)} = 1$ for one-particle states and zero for all others. This is no longer true in an interacting theory because $\Phi(x)$ creates not only one-particle states. In the context of renormalization, we will later absorb $Z_{(1)}$ (which actually turns out to be infinite!) in the definition of the **renormalized field** so that the r.h.s. above becomes $1/(2\pi)^3$; however, this still leaves $Z_{(\lambda)} \neq 0$ for multiparticle states.

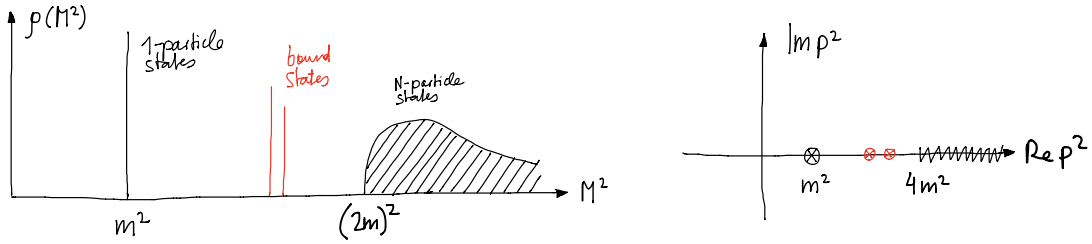

FIGURE 6.2: Left: spectral function of a typical field theory, with a single-particle peak at $M^2 = m^2$ and a multiparticle continuum for $M^2 \geq 4m^2$. Right: Analytic structure of the corresponding dressed propagator with single-particle (and potential bound-state) poles, together with a branch cut above $p^2 = 4m^2$.

For now, we arrive at

$$\langle\Omega|\,\Phi(x)\Phi(y)\,|\Omega\rangle = \frac{1}{(2\pi)^3}\sum_\lambda \int \frac{d^3p}{2E_p(\lambda)}\, e^{-ip(x-y)}\, Z_{(\lambda)}\,. \tag{6.8}$$

Including the time ordering, we can make the same manipulations for the integral as in the free theory, Eqs. (2.84) and (2.86), which leads to

$$\langle\Omega|\,\mathsf{T}\,\Phi(x)\Phi(y)\,|\Omega\rangle = \int \frac{d^4p}{(2\pi)^4}\, e^{-ip(x-y)} \sum_\lambda \frac{iZ_{(\lambda)}}{p^2 - m_\lambda^2 + i\epsilon} = \sum_\lambda Z_{(\lambda)}\, D_F(x-y, m_\lambda^2)\,,$$

where we abbreviated the free Feynman propagator by

$$D_F(z, M^2) := \int \frac{d^4p}{(2\pi)^4}\, e^{-ipz}\, \frac{i}{p^2 - M^2 + i\epsilon}\,. \tag{6.9}$$

Remember that the sum over λ is a multi-dimensional integral over relative momenta. If we further define the **spectral function**

$$\rho(M^2) := \sum_\lambda 2\pi\, \delta(M^2 - m_\lambda^2)\, Z_{(\lambda)}\,, \tag{6.10}$$

then we arrive at the **Källén-Lehmann spectral representation:**

$$\langle\Omega|\,\mathsf{T}\,\Phi(x)\Phi(y)\,|\Omega\rangle = \int_0^\infty \frac{dM^2}{2\pi}\, \rho(M^2)\, D_F(x-y, M^2)\,. \tag{6.11}$$

Therefore, the spectral function encodes the change from a free propagator to a dressed one. The spectral function for a typical theory is positive and has the form of Fig. 6.2. The one-particle states lead to an isolated $\delta-$function peak at $M^2 = m^2$, which allows us to extract the squared mass m^2 of the particle as the **lowest-lying pole location** of the propagator in momentum space:

$$\int d^4x\, e^{ip(x-y)}\, \langle\Omega|\,\mathsf{T}\,\Phi(x)\Phi(y)\,|\Omega\rangle = \frac{iZ}{p^2 - m^2 + i\epsilon} + \int_{4m^2}^\infty \frac{dM^2}{2\pi}\, \frac{i\,\rho(M^2)}{p^2 - M^2 + i\epsilon}\,, \tag{6.12}$$

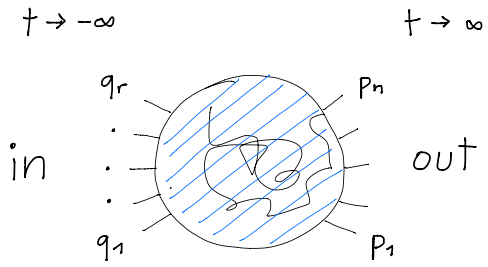

FIGURE 6.3: Idealized scattering process from r incoming to n outgoing particles.

where from now on we write $Z = Z_{(1)}$. The continuum of $N-$particle states begins at $M^2 \geq (2m)^2$, which leads to a branch cut in the propagator starting at $p^2 = 4m^2$. In addition, there could be further bound state poles below $M^2 = (2m)^2$. This property is usually more relevant in the context of composite fields (or higher $n-$point functions of elementary fields) but it can also happen in an elementary two-point function. For example, think of a scalar theory with a Φ^3 interaction: a particle can split into two, which contribute to the two-particle continuum, but in principle they could also form a scalar bound state with mass below $2m$.

S-matrix. The basic observables in scattering experiments are cross sections, which are related to the transition amplitudes that describe the scattering of incoming states $|g, \text{in}\rangle$ to outgoing states $|h, \text{out}\rangle$, cf. Fig. 6.3. Suppose that in the asymptotic past $t \to -\infty$ the state

$$|g, \text{in}\rangle = \int d^3q_1 \ldots \int d^3q_r \, g(\boldsymbol{q}_1, \ldots \boldsymbol{q}_r) \, a^\dagger_{\text{in}}(\boldsymbol{q}_1) \ldots a^\dagger_{\text{in}}(\boldsymbol{q}_r) \, |\Omega\rangle \tag{6.13}$$

describes a collection of wave packets (defined by the function g) that correspond to individual, well-separated single-particle states. When the particles approach each other, they start to interact and scatter into the final state $|h, \text{out}\rangle$, which for $t \to \infty$ describes again asymptotically free and well separated 1-particle states:

$$|h, \text{out}\rangle = \int d^3p_1 \ldots \int d^3p_n \, h(\boldsymbol{p}_1, \ldots \boldsymbol{p}_n) \, a^\dagger_{\text{out}}(\boldsymbol{p}_1) \ldots a^\dagger_{\text{out}}(\boldsymbol{p}_n) \, |\Omega\rangle \, . \tag{6.14}$$

The in and out states are created from the interacting vacuum $|\Omega\rangle$ by action of the fields Φ_{in} and Φ_{out} at $t \to \pm\infty$. These are free fields that satisfy the free Klein-Gordon equation, however with mass $m \neq m_0$, which is the one-particle pole of the Feynman propagator of the full interacting theory, and energy $E_p = \sqrt{\boldsymbol{p}^2 + m^2}$. Therefore, we can expand Φ_{in} and Φ_{out} into Fourier modes with corresponding creation and annihi-

lation operators:

$$\begin{aligned}\Phi_{\text{in}}(x) &= \int \frac{d^3p}{2E_p}\left(a_{\text{in}}(\boldsymbol{p})\, f_p(x) + a^\dagger_{\text{in}}(\boldsymbol{p})\, f_p^*(x)\right),\\ \Phi_{\text{out}}(x) &= \int \frac{d^3p}{2E_p}\left(a_{\text{out}}(\boldsymbol{p})\, f_p(x) + a^\dagger_{\text{out}}(\boldsymbol{p})\, f_p^*(x)\right),\\ f_p(x) &= \frac{1}{(2\pi)^{3/2}}\, e^{-ipx}\Big|_{p^0=E_p}.\end{aligned} \tag{6.15}$$

The question is: how is the full interacting field $\Phi(x)$ related to $\Phi_{\text{in}}(x)$ and $\Phi_{\text{out}}(x)$? What we will need in the following is that

$$\begin{aligned}\langle\alpha|\,\Phi(x)\,|\beta\rangle &\xrightarrow{t\to-\infty} C\,\langle\alpha|\,\Phi_{\text{in}}(x)|\beta\rangle\,,\\ \langle\alpha|\,\Phi(x)\,|\beta\rangle &\xrightarrow{t\to\infty} C\,\langle\alpha|\,\Phi_{\text{out}}(x)|\beta\rangle\,.\end{aligned} \tag{6.16}$$

This does not hold as an operator equation, i.e., the field $\Phi(x)$ does not simply become a free field for $t\to\pm\infty$. The corresponding statement is **Haag's theorem** which says, in short, that a field that is free at a given time remains free for all times. Since we cannot perform measurements with free fields, the corresponding quantum field theory would not have any empirical content. Hence, we only need Eq. (6.16) to hold in the weak sense, i.e., the matrix elements of $\Phi(x)$ should converge to those of $\Phi_{\text{in,out}}(x)$ in a suitable manner at $t\to\pm\infty$. For the overlap of $\Phi(x)$ between the vacuum and one-particle states this entails

$$\underbrace{|\langle\Omega|\,\Phi(0)\,|\lambda_{\boldsymbol{0}}\rangle|^2}_{Z/(2\pi)^3} = C^2\,\underbrace{|\langle\Omega|\,\Phi_{\text{in}}(0)\,|\lambda_{\boldsymbol{0}}\rangle|^2}_{1/(2\pi)^3} \tag{6.17}$$

and therefore $C=\sqrt{Z}$, whereas the (momentum-dependent) overlap with multiparticle states $Z_{(\lambda)}$ must vanish for $t\to\pm\infty$. This can be intuitively understood as follows: although all interactions between the incoming and outgoing particles are switched off asymptotically, the self-interactions of the particles remain, which leads to $m\neq m_0$.

LSZ reduction formula. The operators $\Phi_{\text{in}}(x)$ and $\Phi_{\text{out}}(x)$ act on the same Hilbert space of a free theory. Hence, there must be an operator S (the **scattering operator**) that maps the out states onto the in states: $|g,\text{in}\rangle = S\,|g,\text{out}\rangle$. From this definition it follows that

$$S \text{ is unitary: } S^{-1}=S^\dagger, \qquad S\,|\Omega\rangle=|\Omega\rangle, \qquad \Phi_{\text{in}}(x)=S\,\Phi_{\text{out}}(x)\,S^{-1}. \tag{6.18}$$

The goal in the following will be to compute the transition amplitude or **S-matrix element**

$$\langle h,\text{out}\,|\,g,\text{in}\rangle = \langle h,\text{out}\,|\,S\,|\,g,\text{out}\rangle = \langle h,\text{in}\,|\,S\,|\,g,\text{in}\rangle\,. \tag{6.19}$$

For simplicity we will work directly with the matrix element

$$\langle p_1\ldots p_n,\text{out}\,|\,q_1\ldots q_r,\text{in}\rangle = \langle\Omega\,|\,a_{\text{out}}(\boldsymbol{p}_1)\ldots a_{\text{out}}(\boldsymbol{p}_n)\,a^\dagger_{\text{in}}(\boldsymbol{q}_1)\ldots a^\dagger_{\text{in}}(\boldsymbol{q}_r)\,|\Omega\rangle\,, \tag{6.20}$$

but keep in mind for the following discussion that we should really smear this with normalizable wave packets as in Eqs. (6.13–6.14).

The strategy in calculating the S-matrix element is to successively replace the creation and annihilation operators that appear in Eq. (6.20) by the fully interacting field $\Phi(x)$. To simplify the notation, we return to our definition of the Lorentz-invariant scalar product between fields in Eq. (1.22),

$$(\Psi, \Phi) := i \int d^3x \, \Psi^*(x) \overset{\leftrightarrow}{\partial_0} \Phi(x) = i \int d^3x \left[\Psi^*(x) \dot{\Phi}(x) - \dot{\Psi}^*(x) \Phi(x) \right], \tag{6.21}$$

which is time-independent as long as $\Psi(x)$ and $\Phi(x)$ are solutions of the free Klein-Gordon equation. The relations

$$(f_p, f_{p'}) = 2E_p \, \delta^3(\boldsymbol{p} - \boldsymbol{p}'), \quad (f_p^*, f_{p'}^*) = -2E_p \, \delta^3(\boldsymbol{p} - \boldsymbol{p}'), \quad (f_p, f_{p'}^*) = 0 \tag{6.22}$$

then allow us to extract the Fourier coefficients of Eq. (6.15) as

$$\begin{aligned} a_{\text{in}}(\boldsymbol{p}) &= (f_p, \Phi_{\text{in}}), & a_{\text{out}}(\boldsymbol{p}) &= (f_p, \Phi_{\text{out}}), \\ a_{\text{in}}^\dagger(\boldsymbol{p}) &= -(f_p^*, \Phi_{\text{in}}), & a_{\text{out}}^\dagger(\boldsymbol{p}) &= -(f_p^*, \Phi_{\text{out}}). \end{aligned} \tag{6.23}$$

To begin with, we can write for any function $F(\boldsymbol{x})$:

$$\int_{-\infty}^{\infty} dt \, \frac{\partial}{\partial t} F(\boldsymbol{x}) = \lim_{t \to \infty} F(\boldsymbol{x}) - \lim_{t \to -\infty} F(\boldsymbol{x}). \tag{6.24}$$

Therefore, we can establish the relation

$$\begin{aligned} Z^{-1/2} \int_{-\infty}^{\infty} dt \, \partial_0 \, (f_p, \Phi) &= \lim_{t \to \infty} Z^{-1/2} \, (f_p, \Phi) - \lim_{t \to -\infty} Z^{-1/2} \, (f_p, \Phi) \\ &= (f_p, \Phi_{\text{out}}) - (f_p, \Phi_{\text{in}}) = a_{\text{out}}(\boldsymbol{p}) - a_{\text{in}}(\boldsymbol{p}), \end{aligned} \tag{6.25}$$

where we used Eq. (6.16). Remember that this only holds *inside* expectation values such as that in Eq. (6.20); it is not an operator identity because the identification of $Z^{-1/2} \, \Phi(x)$ with $\Phi_{\text{out}}(x)$, $\Phi_{\text{in}}(x)$ for $t \to \pm\infty$ is only valid in the weak sense. Note that the terms (f_p, Φ_{out}) and (f_p, Φ_{in}) in the second line are time-independent because $\Phi_{\text{out}}(x)$ and $\Phi_{\text{in}}(x)$ solve the Klein-Gordon equation, but (f_p, Φ) depends on time since $\Phi(x)$ is the interacting field. We can then work out its time derivative:

$$\begin{aligned} \partial_0 \, (f_p, \Phi) &= i \int d^3x \, \partial_0 \left[f_p^*(x) \overset{\leftrightarrow}{\partial_0} \Phi(x) \right] \\ &= i \int d^3x \left[f_p^*(x) \, \partial_0^2 \, \Phi(x) - \partial_0^2 \, f_p^*(x) \, \Phi(x) \right], \end{aligned} \tag{6.26}$$

because the crossed terms cancel each other. The idea is now to shuffle the time derivative in the second term from f_p^* to Φ. Since f_p^* is a plane wave, cf. Eq. (6.15), we can convert the time derivative into a spatial derivative:

$$(\partial_0)^2 \, f_p^*(x) = -E_p^2 \, f_p^*(x) = -(\boldsymbol{p}^2 + m^2) \, f_p^*(x) = (\boldsymbol{\nabla}^2 - m^2) \, f_p^*(x). \tag{6.27}$$

At this point we should remember that we will ultimately put this back into the S-matrix element (6.19) that is smeared with wave packets; otherwise the following partial integration cannot be justified because the surface terms would not vanish. In that case we obtain

$$\partial_0 (f_p, \Phi) = i \int d^3x \, f_p^*(x) \, (\partial_0^2 - \boldsymbol{\nabla}^2 + m^2) \, \Phi(x) = i \int d^3x \, f_p^*(x) \, (\Box + m^2) \, \Phi(x) \, . \quad (6.28)$$

In total, Eq. (6.25) becomes

$$a_{\text{out}}(\boldsymbol{p}) = a_{\text{in}}(\boldsymbol{p}) + iZ^{-1/2} \int d^4x \, f_p^*(x) \, (\Box + m^2) \, \Phi(x) \, , \quad (6.29)$$

which again holds only inside the expectation value. Recall that $\Phi(x)$ does *not* satisfy the free Klein-Gordon equation, otherwise the integral would be zero.

Putting this back into the S-matrix element (6.20) and thereby replacing $a_{\text{out}}(\boldsymbol{p}_n)$, we can successively permute $a_{\text{in}}(\boldsymbol{p}_n)$ to the right until it annihilates on the vacuum. Each step generates a factor $2E_{p_n} \, \delta^3(\boldsymbol{p}_n - \boldsymbol{q}_j)$, together with another S-matrix element where two momenta are taken out. Therefore, they describe the scattering of $r-1$ in states into $n-1$ out states. From the perspective of the full S-matrix element they are **disconnected terms**, whereas the connected contribution comes from the second piece in Eq. (6.29):

$$iZ^{-1/2} \int d^4x \, f_p^*(x) \, (\Box + m^2) \, \langle \Omega \, | \, a_{\text{out}}(\boldsymbol{p}_1) \ldots \Phi(x) \, a_{\text{in}}^\dagger(\boldsymbol{q}_1) \, \ldots a_{\text{in}}^\dagger(\boldsymbol{q}_r) \, | \Omega \rangle \, . \quad (6.30)$$

This completes the first step. Next, we want to repeat the procedure for $a_{\text{in}}^\dagger(\boldsymbol{q}_1)$ which appears to the right of $\Phi(x)$. However, in this case it is not sufficient to write $a_{\text{in}}^\dagger(\boldsymbol{q}_1) = a_{\text{out}}^\dagger(\boldsymbol{q}_1) + \ldots$ because ultimately $a_{\text{out}}^\dagger(\boldsymbol{q}_1)$ should annihilate on the left, but we still need to interchange its position with $\Phi(x)$. Earlier we teased that it is the time-ordered propagator (with the Feynman prescription to integrate over poles), and time-ordered correlation functions, that will become important in the interacting theory. In fact, the next step is where the **time ordering** finally comes in:

$$\begin{aligned}
&\Phi(x) \, a_{\text{in}}^\dagger(\boldsymbol{q}) - a_{\text{out}}^\dagger(\boldsymbol{q}) \, \Phi(x) = \\
&\quad = (f_q^*, \Phi_{\text{out}}) \, \Phi(x) - \Phi(x) \, (f_q^*, \Phi_{\text{in}}) \\
&\quad = i \int d^3y \, f_q(y) \overleftrightarrow{\frac{\partial}{\partial y^0}} \Phi_{\text{out}}(y) \, \Phi(x) - i \int d^3y \, f_q(y) \overleftrightarrow{\frac{\partial}{\partial y^0}} \Phi(x) \, \Phi_{\text{in}}(y) \\
&\quad = iZ^{-1/2} \left[\lim_{y^0 \to \infty} \int d^3y \, f_q(y) \overleftrightarrow{\frac{\partial}{\partial y^0}} \Phi(y) \, \Phi(x) - \lim_{y^0 \to -\infty} \int d^3y \, f_q(y) \overleftrightarrow{\frac{\partial}{\partial y^0}} \Phi(x) \, \Phi(y) \right] \\
&\quad = iZ^{-1/2} \int_{-\infty}^{\infty} dy^0 \, \frac{\partial}{\partial y^0} \int d^3y \, f_q(y) \overleftrightarrow{\frac{\partial}{\partial y^0}} \mathsf{T} \, \Phi(x) \, \Phi(y) \\
&\quad = iZ^{-1/2} \int d^4y \, f_q(y) \, (\Box_y + m^2) \, \mathsf{T} \, \Phi(x) \, \Phi(y). \quad (6.31)
\end{aligned}$$

In the third equality we used the fact that the scalar products with Φ_{in} and Φ_{out} are time-independent, so we are free to shift the time variable $y^0 \to \pm\infty$ and replace the interacting field with the in and out fields (which holds inside matrix elements). In the fourth equality we used Eq. (6.24), and we finally repeated the steps that led us from Eq. (6.26) to (6.29). As desired, the second term $a^\dagger_{\text{out}}(\boldsymbol{q})\,\Phi(x)$ on the l.h.s. will produce disconnected terms upon permuting it to the left, whereas the interacting part is generated by the r.h.s. of the equation.

In this way one can proceed until all creation and annihilation operators are replaced by the respective field operators. The final result is

$$\begin{aligned}\langle p_1 \dots p_n, \text{out} \,|\, q_1 \dots q_r, \text{in}\rangle_{\text{conn.}} = (iZ^{-1/2})^{n+r} \left[\prod_{i=1}^{n} \int d^4x_i \, f^*_{p_i}(x_i)\,(\Box_{x_i} + m^2)\right] \times \\ \times \left[\prod_{j=1}^{r} \int d^4y_j \, f_{q_j}(y_j)\,(\Box_{y_j} + m^2)\right] \langle \Omega \,|\mathsf{T}\, \Phi(x_1) \dots \Phi(x_n)\, \Phi(y_1) \dots \Phi(y_r) \,|\Omega\rangle \,.\end{aligned} \tag{6.32}$$

This is known as the **LSZ reduction formula** (Lehmann, Symanzik, Zimmermann). It reduces the computation of S-matrix elements to the calculation of the time-ordered **correlation functions** or simply **Green functions** of the fully interacting theory:

$$G(x_1 \dots x_n, y_1 \dots y_r) := \langle \Omega \,|\mathsf{T}\, \Phi(x_1) \dots \Phi(x_n)\, \Phi(y_1) \dots \Phi(y_r) \,|\Omega\rangle \,. \tag{6.33}$$

For further interpretation, we can use

$$\begin{aligned}\int d^4x \, f^*_p(x)\,(\Box + m^2)\,\Phi(x) &= \int d^4x \,(\Box + m^2)\, f^*_p(x)\,\Phi(x) \\ &= (-p^2 + m^2) \int d^4x \, f^*_p(x)\,\Phi(x)\end{aligned} \tag{6.34}$$

for wave packets, which leads to the following form of the LSZ formula:

$$\begin{aligned}&\prod_{i=1}^{n} \int d^4x_i \, f^*_{p_i}(x_i) \prod_{j=1}^{r} \int d^4y_j \, f_{q_j}(y_j)\, G(x_1 \dots x_n, y_1 \dots y_r) \\ &\quad = \left(\prod_{i=1}^{n} \frac{i\sqrt{Z}}{p_i^2 - m^2}\right) \left(\prod_{j=1}^{r} \frac{i\sqrt{Z}}{q_j^2 - m^2}\right) \langle p_1 \dots p_n, \text{out} \,|\, q_1 \dots q_r, \text{in}\rangle_{\text{conn.}} \,,\end{aligned} \tag{6.35}$$

plus further disconnected terms. The left-hand side is now just the Fourier transform of the Green function, i.e., the Green function in momentum space (modulo factors $(2\pi)^{3/2}$ from the f's). Note that all momenta in the S-matrix element are onshell, $p_i^2 = q_j^2 = m^2$, because these are the physical momenta of 1-particle states. The prefactors on the r.h.s. are therefore singular; they correspond exactly to the pole contributions of the full propagator of the theory, cf. Eq. (6.12). Consequently, they must cancel with the l.h.s.: the Green function will contain a sum of terms with poles in the momenta, where only those terms survive in the connected S-matrix whose poles cancel exactly with the kinematic factors

$$\prod_{i=1}^{n} (p_i^2 - m^2) \prod_{j=1}^{r} (q_j^2 - m^2) \,, \tag{6.36}$$

because all other contributions are not connected. Therefore, the recipe for calculating S-matrix elements is as follows:

- Calculate the Fourier transform of the Green function $G(x_1 \dots x_n, y_1 \dots y_r)$.
- Set all external momenta onshell: $p_i^2 = m^2$, $q_j^2 = m^2$. This generates a sum of terms that are distinguished by their pole structure.
- To obtain the connected S-matrix element, take the residue with respect to the $n + r$ pole factors.

This sounds straightforward enough, but the open question is: how can we actually calculate such Green functions?