The S matrix and the LSZ reduction formula

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The Lehmann–Symanzik–Zimmermann (LSZ) reduction formula makes it possible to calculate the scattering matrix (S matrix) from correlation functions. This note will explain what is meant by in- and out-states, and derive the formula from fundamental assumptions.

1 Eigenstates of interacting theories

We consider an interacting, scalar theory with field $\phi(x)$, describing particles with mass. The Hamilton operator of the full (interacting) theory is H, and the momentum operator is $\mathbf{P}$. The theory is assumed to obey Poincaré symmetry, and has the following properties:

1. There is a unique and Poincaré-invariant (translational and Lorentz invariant) vacuum state $|\Omega\rangle$. The energy scale is chosen such that the vacuum state has zero energy, $H|\Omega\rangle = 0$.

2. Vanishing field vacuum expectation value: $\langle\Omega|\phi(0)|\Omega\rangle = 0$.

In Peskin and Schroeder p. 212, it is stated that assumption 2 is usually satisfied by symmetry; for higher-spin fields it is zero by Lorentz invariance. Other authors (e.g. Srednicki) suggest that if $\langle\Omega|\phi(0)|\Omega\rangle \equiv C \neq 0$, we can redefine the field by subtracting C. This will, of course, lead to another Lagrangian. For ϕ^4-theory, $\langle\Omega|\phi(0)|\Omega\rangle = 0$ can be established with the usual approach to calculate correlation functions (where one of the two functions is $\phi(0)$ and the other is the identity) (problem set 8, problem 1). This is because Wick's theorem leads to zero vacuum expectation value for any odd numbers of fields.

Note that in addition to the first assumption, we also have $H_0|0\rangle = 0$, for the free Hamiltonian H_0 and the free vacuum state $|0\rangle$. This property is viewed as a result of a choice during quantization. Indeed there is an ordering ambiguity when expressing the classical, free Hamiltonian before promoting the fields to operators. For example, a single harmonic oscillator of unit mass has energy

$$\frac{p^2}{2} + \frac{1}{2}\omega^2 q^2 = \frac{1}{2}(\omega q - ip)(\omega q + ip). \tag{1}$$

When using the expression on the left-hand side as the Hamiltonian, we obtain $\omega(a^\dagger a + \frac{1}{2})$ after quantization, while when using the right-hand side we get only

$\omega a^\dagger a$. The ordering ambiguity can therefore justify a free-field Hamiltonian H_0 with the property $H_0|0\rangle = 0$.

From Poincaré symmetry we can prove (problem set 4, problem 3)

$$[H, \mathbf{P}] = 0. \tag{2}$$

Thus we take $|\lambda_\mathbf{p}\rangle$ to be common eigenstates of $\mathbf{P}$ and H with momentum $\mathbf{p}$ and energy $E^\lambda_\mathbf{p}$. Define $m_\lambda = E^\lambda_\mathbf{p}\big|_{\mathbf{p}=0}$ to be the rest energy (mass) of the states. Note that the states do not necessarily describe single particles (see Fig. 1).

Consider a Lorentz transformation Λ that takes the four-vector $(m_\lambda, 0)$ to $p^\mu = (p^0, \mathbf{p})$, where $(p^0)^2 = \mathbf{p}^2 + m^2_\lambda$. The Lorentz transformation is described by a unitary operator U on the quantum states. From Poincaré symmetry we have (problem set 4, problem 3)

$$U^\dagger P^\mu U = \Lambda^\mu{}_\nu P^\nu. \tag{3}$$

Thus

$$P^\mu U|\lambda_0\rangle = UU^\dagger P^\mu U|\lambda_0\rangle = U\Lambda^\mu{}_\nu P^\nu|\lambda_0\rangle = U\Lambda^\mu{}_0 m_\lambda|\lambda_0\rangle = p^\mu U|\lambda_0\rangle, \tag{4a}$$

$$\begin{aligned} P^\mu U^\dagger|\lambda_\mathbf{p}\rangle &= U^\dagger U P^\mu U^\dagger|\lambda_\mathbf{p}\rangle = U^\dagger(\Lambda^{-1})^\mu{}_\nu P^\nu|\lambda_\mathbf{p}\rangle \\ &= U^\dagger(\Lambda^{-1})^\mu{}_\nu p^\nu|\lambda_\mathbf{p}\rangle = \delta^\mu_0 m_\lambda U^\dagger|\lambda_\mathbf{p}\rangle, \end{aligned} \tag{4b}$$

In other words, $U|\lambda_0\rangle$ is an eigenstate of P^μ with eigenvalue p^μ, and $U^\dagger|\lambda_\mathbf{p}\rangle$ is an eigenstate of P^μ with eigenvalue $(m_\lambda, 0)$. Due to this one-to-one correspondence through the Lorentz transformation Λ, we may identify $U|\lambda_0\rangle \equiv |\lambda_\mathbf{p}\rangle$. Moreover the energy eigenvalue of $|\lambda_\mathbf{p}\rangle$ is

$$E^\lambda_\mathbf{p} = \sqrt{\mathbf{p}^2 + m^2_\lambda}, \tag{5}$$

see Fig. 1. For the special case where λ denotes a single particle, we write $|\mathbf{p}\rangle$ rather than $|\lambda_\mathbf{p}\rangle$.

From Poincaré symmetry (problem set 4, problem 3), we know that translations by x^μ in spacetime is implemented by the unitary operator $e^{-iPx} = e^{-P_\mu x^\mu}$ on the quantum states, and that

$$\phi(x) = e^{iPx}\phi(0)e^{-iPx}. \tag{6}$$

The assumption 2 above therefore means that

$$\langle\Omega|\phi(x)|\Omega\rangle = \langle\Omega|e^{iPx}\phi(0)e^{-iPx}|\Omega\rangle = \langle\Omega|\phi(0)|\Omega\rangle = 0. \tag{7}$$

The second equality results from the translational invariance of the vacuum state (assumption 1).

We also have

$$\begin{aligned} \langle\Omega|\phi(x)|\lambda_\mathbf{p}\rangle &= \langle\Omega|e^{iPx}\phi(0)e^{-iPx}|\lambda_\mathbf{p}\rangle = \langle\Omega|\phi(0)|\lambda_\mathbf{p}\rangle e^{-ipx} \\ &= \langle\Omega|UU^\dagger\phi(0)U|\lambda_0\rangle e^{-ipx} = \langle\Omega|U^\dagger\phi(0)U|\lambda_0\rangle e^{-ipx} \\ &= \langle\Omega|\phi(0)|\lambda_0\rangle e^{-ipx}, \quad p^0 = E^\lambda_\mathbf{p} = \sqrt{\mathbf{p}^2 + m^2_\lambda}, \end{aligned} \tag{8}$$

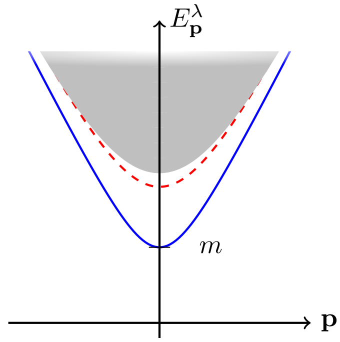

Figure 1: Energy of the eigenstates as a function of momentum. The rest energy of the single particle state (blue curve) is denoted m. From $2m$ and above there is a continuum of multiparticle states (gray area): Note that a two-particle state can have any energy above $2m$ even though their total momentum is zero (since the individual particles may still move). In some theories there may also be bound states of two particles, shown as a red, dashed curve slightly below the two-particle continuum of free particles.

where the last equality results since $\phi(0)$ is a Lorentz scalar. The absolute square of the last inner product, in the special case where λ denotes a single particle, will be denoted Z:

$$Z = |\langle\Omega|\phi(0)|\mathbf{p}=0\rangle|^2. \tag{9}$$

We may assume that $\langle\Omega|\phi(0)|\lambda_0\rangle$ is positive, by absorbing a suitable phase factor into the state $|\lambda_0\rangle$. Then the absolute value may be omitted from (9):

$$Z = \langle\Omega|\phi(0)|\mathbf{p}=0\rangle^2. \tag{10}$$

2 Defining in- and out-states

To consider scattering experiments, we need to form wavepacket states with spectra $\psi(\mathbf{k}-\mathbf{p}_i)$ centered about the input (or output) momenta $\mathbf{p}_i$, $i = 1, 2, \ldots$ For simplicity we will let $\psi(\mathbf{k})$ be for example a gaussian centered about $\mathbf{k} = 0$, such that the spectrum $\psi(\mathbf{k}-\mathbf{p}_i)$ is centered about $\mathbf{k} = \mathbf{p}_i$. The wavepackets make the states localized such that they do not interact with each other for asymptotic times $t \to \pm\infty$. This is necessary to establish the S matrix and the LSZ formula. Once the job is done, we may go to the plane-wave limit of infinitely narrow spectra about the $\mathbf{p}_i$'s.

One may think that in the asymptotic limits $t \to \pm\infty$ the field is free, and one may simply use the single particle states of the free theory. However, it is important to be aware of that the interaction does not go away even in the asymptotic limit. In ϕ^4 theory a single particle experiences self-interaction, and in QED an electron will always be together with its photon cloud (electromagnetic field).

2.1 Free field wave packets

In the free Klein-Gordon theory we may define wavepacket single particle states

$$\left|\mathbf{p}^\psi\right\rangle = \sqrt{2E_\mathbf{p}}\, a_\mathbf{p}^{\psi\dagger}|0\rangle, \quad a_\mathbf{p}^{\psi\dagger} = \int \frac{d^3k}{(2\pi)^3}\psi(\mathbf{k}-\mathbf{p})a_\mathbf{k}^\dagger. \tag{11}$$

We have

$$\begin{aligned}\langle 0|\phi(x)\frac{\left|\mathbf{p}^\psi\right\rangle}{\sqrt{2E_\mathbf{p}}} &= \langle 0|\int \frac{d^3q}{(2\pi)^3}\frac{1}{\sqrt{2E_\mathbf{q}}}\left(a_\mathbf{q}e^{-iqx} + a_\mathbf{q}^\dagger e^{iqx}\right)\int \frac{d^3k}{(2\pi)^3}\psi(\mathbf{k}-\mathbf{p})a_\mathbf{k}^\dagger|0\rangle \\ &= \int \frac{d^3k}{(2\pi)^3}\frac{\psi(\mathbf{k}-\mathbf{p})}{\sqrt{2E_\mathbf{k}}}e^{-ikx}, \end{aligned}\tag{12}$$

so it is natural to define a wave function by

$$\Psi_\mathbf{p}(x) = \int \frac{d^3k}{(2\pi)^3}\frac{\psi(\mathbf{k}-\mathbf{p})}{\sqrt{2E_\mathbf{k}}}e^{-ikx}, \quad k^0 = E_\mathbf{k} = \sqrt{\mathbf{k}^2 + m_0^2}, \tag{13}$$

with the free (or "bare") mass m_0. In (11) and (13) we have used a subscript $\mathbf{p}$ to indicate that the spectrum is centered about $\mathbf{p}$.

As can be verified directly, we can determine the ladder operators from the field by

$$a_\mathbf{p}^\psi = i\int d^3x\,\Psi_\mathbf{p}^*(x)\overleftrightarrow{\partial}_0\phi(x), \tag{14}$$

where the operation $\overleftrightarrow{\partial}_0$ is defined by

$$f\overleftrightarrow{\partial}_0 g = f\partial_0 g - (\partial_0 f)g. \tag{15}$$

Note that even though $\Psi_\mathbf{p}(x)$ and $\phi(x)$ are dependent on time, the result in (14) is independent of time. (For more details and intuition about free field wave packets, see problem set 3. For a detailed derivation of (14) in a special case, see problem set 2, problem 2.)

2.2 Wavepackets and operators for interacting fields

For interacting fields we define

$$\left|\lambda_\mathbf{p}^\psi\right\rangle = \int \frac{d^3k}{(2\pi)^3}\psi(\mathbf{k}-\mathbf{p})|\lambda_\mathbf{k}\rangle, \tag{16a}$$

$$\left|\mathbf{p}^\psi\right\rangle = \int \frac{d^3k}{(2\pi)^3}\psi(\mathbf{k}-\mathbf{p})|\mathbf{k}\rangle. \tag{16b}$$

Here (16a) describes a wavepacket constructed from the arbitrary eigenstate $|\lambda_{\mathbf{p}}\rangle$, while (16b) describe a single particle.

Furthermore we *define* operators

$$a^{\psi}_{\mathbf{p}}(t) = i\int d^3x \Psi^*_{\mathbf{p}}(x)\overleftrightarrow{\partial}_0\phi(x), \tag{17a}$$

$$a^{\psi\dagger}_{\mathbf{p}}(t) = -i\int d^3x \Psi_{\mathbf{p}}(x)\overleftrightarrow{\partial}_0\phi(x), \tag{17b}$$

where

$$\Psi_{\mathbf{p}}(x) = \int \frac{d^3k}{(2\pi)^3}\frac{\psi(\mathbf{k}-\mathbf{p})}{\sqrt{2E_{\mathbf{k}}}}e^{-ikx}, \quad k^0 = E_{\mathbf{k}} = \sqrt{\mathbf{k}^2+m^2}, \tag{18}$$

with the single particle mass m in the interacting theory. The time dependence of (17) is not of the Heisenberg type; this is demonstrated by the fact that there is no time dependence at all in the free-field special case (according to (14)). In general these operators have complicated properties, but we will consider them in the limits $t \to \pm\infty$. Then they turn out to be similar to the usual ladder operators, as long as we consider the first two steps of the ladder only (vacuum and single particle states).

2.3 Properties of $a^{\psi}_{\mathbf{p}}(t)$ and $a^{\psi\dagger}_{\mathbf{p}}(t)$

From (7) and (17) we obtain

$$\langle\Omega|a^{\psi}_{\mathbf{p}}(t)|\Omega\rangle = \langle\Omega|a^{\psi\dagger}_{\mathbf{p}}(t)|\Omega\rangle = 0. \tag{19}$$

Furthermore, (16), (17), (8), and (18) lead to

$$\begin{aligned}
\langle\Omega|a^{\psi}_{\mathbf{q}}(t)\big|\lambda^{\psi}_{\mathbf{p}}\rangle &= i\int d^3x\Psi^*_{\mathbf{q}}(x)\overleftrightarrow{\partial}_0\int\frac{d^3k}{(2\pi)^3}\psi(\mathbf{k}-\mathbf{p})\langle\Omega|\phi(x)|\lambda_{\mathbf{k}}\rangle\\
&= \langle\Omega|\phi(0)|\lambda_0\rangle\int\frac{d^3k}{(2\pi)^3}\psi(\mathbf{k}-\mathbf{p})\int d^3x\Psi^*_{\mathbf{q}}(x)i\overleftrightarrow{\partial}_0 e^{-ikx}\Big|_{k^0=E^{\lambda}_{\mathbf{k}}=\sqrt{\mathbf{k}^2+m^2_{\lambda}}}\\
&= \langle\Omega|\phi(0)|\lambda_0\rangle\int\frac{d^3k}{(2\pi)^3}\int\frac{d^3k'}{(2\pi)^3}\psi(\mathbf{k}-\mathbf{p})\frac{\psi^*(\mathbf{k}'-\mathbf{q})}{\sqrt{2E_{\mathbf{k}'}}}\int d^3x e^{ik'x}i\overleftrightarrow{\partial}_0 e^{-ikx}\Big|_{k^0=E^{\lambda}_{\mathbf{k}}\text{ and }k'^0=E_{\mathbf{k}'}}\\
&= \langle\Omega|\phi(0)|\lambda_0\rangle\int\frac{d^3k}{(2\pi)^3}\int\frac{d^3k'}{(2\pi)^3}\psi(\mathbf{k}-\mathbf{p})\psi^*(\mathbf{k}'-\mathbf{q})\frac{E^{\lambda}_{\mathbf{k}}+E_{\mathbf{k}'}}{\sqrt{2E_{\mathbf{k}'}}}e^{i(E_{\mathbf{k}'}-E^{\lambda}_{\mathbf{k}})t}(2\pi)^3\delta(\mathbf{k}-\mathbf{k}')\\
&= \langle\Omega|\phi(0)|\lambda_0\rangle\int\frac{d^3k}{(2\pi)^3}\psi(\mathbf{k}-\mathbf{p})\psi^*(\mathbf{k}-\mathbf{q})\frac{E^{\lambda}_{\mathbf{k}}+E_{\mathbf{k}}}{\sqrt{2E_{\mathbf{k}}}}e^{i(E_{\mathbf{k}}-E^{\lambda}_{\mathbf{k}})t}.
\end{aligned} \tag{20}$$

By letting $t\to\infty$ this tends to zero, except when $E_{\mathbf{k}} - E^{\lambda}_{\mathbf{k}} = 0$, that is, when λ corresponds to a single particle state. This happens because the rapid oscillation of the exponential washes out the integral (Riemann-Lebesgue lemma)[1]. If we

[1] There seems to be a complication as $|\mathbf{k}|\to\infty$ in the integral, because then $E_{\mathbf{k}} - E^{\lambda}_{\mathbf{k}} \to 0$. However we eliminate this problem by choosing a spectrum $\psi(\mathbf{k})$ which tends sufficiently fast to zero, or even has finite support.

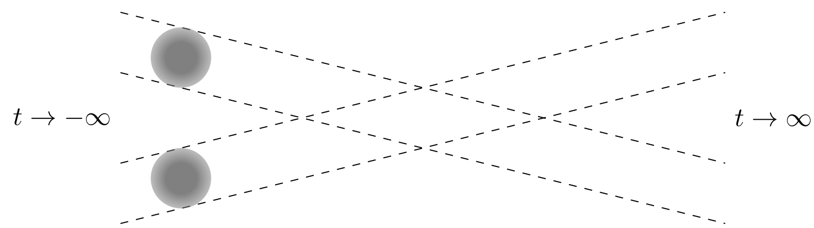

Figure 2: Two beams. When $t \to \pm\infty$ the particles are spatially separated. The gray balls represent $|\Psi_{\mathbf{p}}(x)|^2$ (see (18)) for two different $\mathbf{p}$'s, and for a large negative t. Thus they visualize the wave function associated with the in-state. The dashed lines show the direction of the beams in the case with negligible interaction; in general the scattered beams may have different directions than the incoming beams (and there may be more than two outgoing particles).

now let $\psi(\mathbf{k})$ be sufficiently narrow,

$$\psi(\mathbf{k}) \to (2\pi)^3\delta(\mathbf{k}), \tag{21}$$

we obtain

$$\langle\Omega|a_{\mathbf{q}}(\pm\infty)|\lambda_{\mathbf{p}}\rangle = \langle\lambda_{\mathbf{p}}|a^\dagger_{\mathbf{q}}(\pm\infty)|\Omega\rangle = \begin{cases} \sqrt{Z}\sqrt{2E_{\mathbf{p}}}(2\pi)^3\delta(\mathbf{p}-\mathbf{q}), & \lambda = \text{single particle}, \\ 0, & \text{else}. \end{cases} \tag{22}$$

Here we have used (10). Since we have used the plane-wave limit (21) we have omitted the superscript ψ in (22); however, one should have in mind that the plane-wave limit can only be taken after the $t \to \pm\infty$ limit.

By a similar calculation we find

$$\langle\lambda_{\mathbf{p}}|a_{\mathbf{q}}(\pm\infty)|\Omega\rangle = \langle\Omega|a^\dagger_{\mathbf{q}}(\pm\infty)|\lambda_{\mathbf{p}}\rangle = 0. \tag{23}$$

Since $|\lambda_{\mathbf{p}}\rangle$ for all λ and $\mathbf{p}$, and $|\Omega\rangle$, span the entire Hilbert space (they are the eigenstates of the hermitian operator H), (19), (22), and (23) imply that

$$|\mathbf{p}\rangle = \frac{\sqrt{2E_{\mathbf{p}}}}{\sqrt{Z}}a^\dagger_{\mathbf{p}}(\pm\infty)|\Omega\rangle, \tag{24}$$

and that

$$a_{\mathbf{p}}(\pm\infty)|\Omega\rangle = 0. \tag{25}$$

Moreover, since $\Psi_{\mathbf{p}}(x)$ and $\Psi_{\mathbf{q}}(x)$ are spatially separated for sufficiently large $|t|$, we have

$$\left[a^{\psi}_{\mathbf{p}}(t), a^{\psi\dagger}_{\mathbf{q}}(t)\right] = 0, \quad \mathbf{p} \neq \mathbf{q}, \quad t \to \pm\infty, \tag{26}$$

and therefore

$$\left[a_{\mathbf{p}}(\pm\infty), a^\dagger_{\mathbf{q}}(\pm\infty)\right] = 0, \quad \mathbf{p} \neq \mathbf{q}, \tag{27}$$

provided we take the limit $t \to \pm\infty$ before the plane-wave limit.

We may now form the asymptotic in- and out-states:

$$|\mathbf{k}_1\mathbf{k}_2\cdots\rangle_{\text{in}} = \prod_i \frac{\sqrt{2E_{\mathbf{k}_i}}}{\sqrt{Z}} a^\dagger_{\mathbf{k}_i}(-\infty)|\Omega\rangle, \tag{28a}$$

$$|\mathbf{p}_1\mathbf{p}_2\cdots\rangle_{\text{out}} = \prod_j \frac{\sqrt{2E_{\mathbf{p}_j}}}{\sqrt{Z}} a^\dagger_{\mathbf{p}_j}(\infty)|\Omega\rangle. \tag{28b}$$

Note that the in-state and out-state in (28) are independent of time, and live in the Heisenberg picture, with the same reference time. In the limit of negligible interaction they are equal. Thus the propagation of the wavepacket particles in time and space is *not* described by the argument t in the ladder operators $a^{\psi\dagger}_{\mathbf{k}_i}(t)$. Instead, the propagation is described with expectation values of operators/observables in the usual way. For example, in the free theory we have $\langle \mathbf{p}^\psi | N\phi^2(x) | \mathbf{p}^\psi \rangle = 4E_{\mathbf{p}}|\Psi_{\mathbf{p}}(x)|^2$, where $\Psi_{\mathbf{p}}(x)$ is given by (13) and propagates according to the Klein-Gordon wave equation with the bare mass m_0. Similarly to (12)-(13) in the free field case, we may use (8), (10), and (16b) to identify a wave function in the interacting case,

$$\frac{1}{\sqrt{Z}}\langle\Omega|\phi(x)\frac{|\mathbf{p}^\psi\rangle}{\sqrt{2E_{\mathbf{p}}}} = \Psi_{\mathbf{p}}(x), \tag{29}$$

with $\Psi_{\mathbf{p}}(x)$ given by (18). The wave function satisfies the Klein-Gordon equation with the physical mass m in this case (where we only have a single particle). We may define wave functions when more particles are present also, but the behavior will generally be complicated since the multiparticle states are not necessarily eigenstates of the total Hamiltonian. Physically this means the particles may collide and undergo a complicated evolution.

We may also consider the scattering in the Schrödinger picture. Let $t = -T$ be the far past when the particles are well separated (see Fig. 2), and $t = T$ is the far future. The time evolution operator in the Schrödinger picture, connecting far past to far future, is $S \equiv e^{-iH2T}$. We let states with subscripts "in" or "out" be in the Heisenberg picture, while states without these subscripts are in the Schrödinger picture. The reference time for the pictures is taken to be $t = -T$. Then

$$\begin{aligned} {}_{\text{out}}\langle\mathbf{p}_1\mathbf{p}_2\cdots|\mathbf{k}_1\mathbf{k}_2\cdots\rangle_{\text{in}} &= {}_{\text{out}}\langle\mathbf{p}_1\mathbf{p}_2\cdots|S^\dagger S|\mathbf{k}_1\mathbf{k}_2\cdots\rangle_{\text{in}} \\ &= \langle\mathbf{p}_1\mathbf{p}_2\cdots|S|\mathbf{k}_1\mathbf{k}_2\cdots\rangle, \end{aligned} \tag{30}$$

where $|\mathbf{k}_1\mathbf{k}_2\cdots\rangle = |\mathbf{k}_1\mathbf{k}_2\cdots\rangle_{\text{in}}$ is the Schrödinger-picture counterpart at $t = -T$ of the in-state, and $\langle\mathbf{p}_1\mathbf{p}_2\cdots| = {}_{\text{out}}\langle\mathbf{p}_1\mathbf{p}_2\cdots|S^\dagger$ is the Schrödinger-picture counterpart at $t = T$ of the out-state. Eq. (30) explains why the numbers ${}_{\text{out}}\langle\mathbf{p}_1\mathbf{p}_2\cdots|\mathbf{k}_1\mathbf{k}_2\cdots\rangle_{\text{in}}$ are called S matrix elements.

The S matrix (or the related $\mathcal{M}$ matrix, see Sec. 4) has important relevance in scattering or collision experiments, and decay rates. It describes the probability amplitudes of outgoing particles with given momenta, for a given set of incoming particles and momenta.

3 LSZ reduction

Rather than (28) we initially keep the wavepacket version of the ladder operators:

$$|\mathbf{k}_1\mathbf{k}_2\cdots\rangle_{\text{in}} \equiv |\text{in}\rangle = \prod_i \frac{\sqrt{2E_{\mathbf{k}_i}}}{\sqrt{Z}} a^{\psi\dagger}_{\mathbf{k}_i}(-\infty)|\Omega\rangle, \tag{31a}$$

$$|\mathbf{p}_1\mathbf{p}_2\cdots\rangle_{\text{out}} \equiv |\text{out}\rangle = \prod_j \frac{\sqrt{2E_{\mathbf{p}_j}}}{\sqrt{Z}} a^{\psi\dagger}_{\mathbf{p}_j}(\infty)|\Omega\rangle. \tag{31b}$$

For simplicity we consider only two particles in the in-state (the generalization is straightforward). The S matrix elements are then given by

$$\langle\text{out}|\text{in}\rangle = A\langle\text{out}|a^{\psi\dagger}_{\mathbf{k}_1}(-\infty)a^{\psi\dagger}_{\mathbf{k}_2}(-\infty)|\Omega\rangle, \tag{32}$$

where

$$A = \sqrt{2E_{\mathbf{k}_1}}\sqrt{2E_{\mathbf{k}_2}}/\sqrt{Z}^2. \tag{33}$$

We have

$$\langle\text{out}|a^{\psi\dagger}_{\mathbf{k}_1}(-\infty)a^{\psi\dagger}_{\mathbf{k}_2}(-\infty)|\Omega\rangle = \langle\text{out}|\Big[a^{\psi\dagger}_{\mathbf{k}_1}(-\infty) - a^{\psi\dagger}_{\mathbf{k}_1}(\infty)\Big]a^{\psi\dagger}_{\mathbf{k}_2}(-\infty)|\Omega\rangle, \tag{34}$$

provided $a^{\psi\dagger}_{\mathbf{k}_1}(\infty)$ commutes with all ladder operators in $\langle\text{out}|$, that is, with $a^{\psi}_{\mathbf{p}_j}(\infty)$ for all j. This is the case as long as $\mathbf{k}_1 \neq \mathbf{p}_j$ for all j. We assume this is the case. Later we must also assume that $\mathbf{k}_2 \neq \mathbf{p}_j$ for all j. In other words, we will be able to calculate almost all S matrix elements except the ones with $\mathbf{p}_j$ exactly equal to $\mathbf{k}_{1,2}$ for some j (but we may come arbitrarily close). This means that in particular we do not obtain the trivial part of the S matrix where the in- and out-states are equal.

With the help of (17) this gives

$$\langle\text{out}|\text{in}\rangle = iA\left[\lim_{t_1\to\infty} - \lim_{t_1\to-\infty}\right]\int d^3x_1 \Psi_{\mathbf{k}_1}(x_1)\overset{\leftrightarrow x_1}{\partial_0}\langle\text{out}|\phi(x_1)a^{\psi\dagger}_{\mathbf{k}_2}(-\infty)|\Omega\rangle, \tag{35}$$

where the superscript x_1 in $\overset{\leftrightarrow x_1}{\partial_0}$ means that the operator acts on x_1. For any functions $f(x)$ and $g(x)$, where $f(x)$ satisfies the Klein-Gordon equation, and tends sufficiently fast to zero as $|\mathbf{x}| \to \infty$ (a gaussian is more than sufficient), we have

$$\begin{aligned}
&\left[\lim_{t\to\infty} - \lim_{t\to-\infty}\right]\int d^3x f(x)\overset{\leftrightarrow}{\partial}_0 g(x) = \int d^4x \partial_0\Big(f(x)\overset{\leftrightarrow}{\partial}_0 g(x)\Big) \\
&= \int d^4x\big[f(x)\partial_0^2 g(x) - (\partial_0^2 f(x))g(x)\big] \\
&= \int d^4x\big[f(x)\partial_0^2 g(x) + \big[(m^2 - \nabla^2)f(x)\big)\big]g(x)\big] \\
&= \int d^4x f(x)\big(\Box + m^2\big)g(x).
\end{aligned} \tag{36}$$

In the last step we have use integration by parts twice, to move the ∇^2 from $f(x)$ to $g(x)$. The associated surface terms vanish when $f(x)$ tends sufficiently fast to zero in 3D space for fixed x^0. Using (36) in (35) we are done with the first reduction:

$$\langle \text{out}|\text{in}\rangle = iA \int d^4x_1 \Psi_{\mathbf{k}_1}(x_1)(\Box_{x_1} + m^2)\langle \text{out}|\phi(x_1)a^{\psi\dagger}_{\mathbf{k}_2}(-\infty)|\Omega\rangle. \tag{37}$$

With this first step, we have effectively got rid of the first ladder operator. In the next step, it is time to get rid of the next ladder operator:

$$\begin{aligned}
&\langle \text{out}|\phi(x_1)a^{\psi\dagger}_{\mathbf{k}_2}(-\infty)|\Omega\rangle = \langle \text{out}|\phi(x_1)a^{\psi\dagger}_{\mathbf{k}_2}(-\infty)|\Omega\rangle - \langle \text{out}|a^{\psi\dagger}_{\mathbf{k}_2}(\infty)\phi(x_1)|\Omega\rangle \\
&= i\left[\lim_{t_2\to\infty} - \lim_{t_2\to-\infty}\right] \int d^3x_2 \Psi_{\mathbf{k}_2}(x_2)\overset{\leftrightarrow x_2}{\partial_0} \langle \text{out}|T\phi(x_1)\phi(x_2)|\Omega\rangle \\
&= i \int d^4x_2 \Psi_{\mathbf{k}_2}(x_2)(\Box_{x_2} + m^2)\langle \text{out}|T\phi(x_1)\phi(x_2)|\Omega\rangle.
\end{aligned} \tag{38}$$

Continuing this way, we get rid of all ladder operators in $\langle \text{out}|$ also. The result is

$$\begin{aligned}
\langle \text{out}|\text{in}\rangle = &\prod_i \frac{i\sqrt{2E_{\mathbf{k}_i}}}{\sqrt{Z}} \int d^4x_i \Psi_{\mathbf{k}_i}(x_i)(\Box_{x_i} + m^2) \\
&\cdot \prod_j \frac{i\sqrt{2E_{\mathbf{p}_j}}}{\sqrt{Z}} \int d^4y_j \Psi^*_{\mathbf{p}_j}(y_j)(\Box_{y_j} + m^2) \\
&\cdot \langle \Omega|T\phi(x_1)\phi(x_2)\cdots\phi(y_1)\phi(y_2)\cdots|\Omega\rangle.
\end{aligned} \tag{39}$$

Taking the plane-wave limit (21), which implies $\Psi_{\mathbf{k}}(x) \to \frac{1}{\sqrt{2E_{\mathbf{k}}}} e^{-ikx}$, we obtain the LSZ reduction formula

$$\begin{aligned}
\langle \text{out}|\text{in}\rangle = &\prod_i \frac{i}{\sqrt{Z}} \int d^4x_i e^{-ik_ix_i}(\Box_{x_i} + m^2) \\
&\cdot \prod_j \frac{i}{\sqrt{Z}} \int d^4y_j e^{ip_jy_j}(\Box_{y_j} + m^2) \\
&\cdot \langle \Omega|T\phi(x_1)\phi(x_2)\cdots\phi(y_1)\phi(y_2)\cdots|\Omega\rangle.
\end{aligned} \tag{40}$$

If $G(k)$ is the Fourier transform of $g(x)$, then $-k^2G(k)$ is the Fourier transform of $\Box g(x)$. This leads to the alternative and final form of the LSZ reduction formula for the S matrix elements (assuming $\mathbf{k}_i \neq \mathbf{p}_j$):

$$\begin{aligned}
\langle \mathbf{p}_1\mathbf{p}_2\cdots|S|\mathbf{k}_1\mathbf{k}_2\cdots\rangle &= {}_{\text{out}}\langle \mathbf{p}_1\mathbf{p}_2\cdots|\mathbf{k}_1\mathbf{k}_2\cdots\rangle_{\text{in}} \\
&= \prod_i \frac{k_i^2 - m^2}{i\sqrt{Z}} \int d^4x_i e^{-ik_ix_i} \\
&\cdot \prod_j \frac{p_j^2 - m^2}{i\sqrt{Z}} \int d^4y_j e^{ip_jy_j} \\
&\cdot \langle \Omega|T\phi(x_1)\phi(x_2)\cdots\phi(y_1)\phi(y_2)\cdots|\Omega\rangle.
\end{aligned} \tag{41}$$

The LSZ reduction formula (41) is also given in Peskin and Schroeder (7.42). It expresses the S matrix elements as a Fourier transform of the correlation function

$$\langle\Omega|T\phi(x_1)\phi(x_2)\cdots\phi(y_1)\phi(y_2)\cdots|\Omega\rangle, \tag{42}$$

multiplied by factors $(k_i^2-m^2)/i\sqrt{Z}$ and $(p_j^2-m^2)/i\sqrt{Z}$. These factors eliminate corresponding poles in the Fourier transformed diagrams of (42). If any of these poles is missing from a particular diagram, one gets zero as the external particles go on mass shell $k_i^2=m^2$ and $p_j^2=m^2$.

With the LSZ formula we have a method for obtaining the S matrix from a correlation function, which in turn can be calculated as a sum of connected Feynman diagrams. Since the correlation function is Fourier transformed in (41), the diagrams must be Fourier transformed.

4 Connected and amputated diagrams

Fourier transforming the diagrams of correlation functions is achieved by omitting the exponential factors of external points, and associated momentum integrals, from the momentum-space Feynman rules. This can be done for all external points except those where the momentum is determined by the other external momenta.

Consider, for example, the diagram in Fig. 3. Applying the momentum-space Feynman rules (Peskin & Schroeder p. 95) we obtain

$$\begin{aligned}
&\langle\Omega|T\phi(x_1)\phi(x_2)\phi(y_1)\phi(y_2)|\Omega\rangle\\
=&(-i\lambda)\int\frac{d^4k_1}{(2\pi)^4}e^{ik_1x_1}\int\frac{d^4k_2}{(2\pi)^4}e^{ik_2x_2}\int\frac{d^4p_1}{(2\pi)^4}e^{-ip_1y_1}e^{-i(k_1+k_2-p_1)y_2}\\
&\cdot D_F(k_1)D_F(k_2)D_F(p_1)D_F(k_1+k_2-p_1),
\end{aligned} \tag{43}$$

where $D_F(p)$ is the Feynman propagator in momentum space. Note that since $p_2=k_1+k_2-p_1$, the Feynman rules don't imply integration with respect to p_2. The Fourier transforms with respect to k_1, k_2, and p_1 are taken simply by omitting the corresponding exponential factors and integrals. The last Fourier transform (with respect to y_2) gives a delta function $(2\pi)^4\delta(k_1+k_2-p_1-p_2)$. Thus

$$\begin{aligned}
&\int d^4x_1e^{-ik_1x_1}\int d^4x_2e^{-ik_2x_2}\int d^4y_1e^{ip_1y_1}\int d^4y_2e^{ip_2y_2}\langle\Omega|T\phi(x_1)\phi(x_2)\phi(y_1)\phi(y_2)|\Omega\rangle\\
&=(-i\lambda)(2\pi)^4\delta(k_1+k_2-p_1-p_2)D_F(k_1)D_F(k_2)D_F(p_1)D_F(k_1+k_2-p_1).
\end{aligned} \tag{44}$$

Due to the overall momentum conserving delta function [$\delta(k_1+k_2-p_1-p_2)$ in (44)], we define $\mathcal{M}$ by

$$\langle\mathbf{p}_1\mathbf{p}_2\cdots|S|\mathbf{k}_1\mathbf{k}_2\cdots\rangle = i\mathcal{M}(\mathbf{k}_1,\mathbf{k}_2,\ldots,\mathbf{p}_1,\mathbf{p}_2,\ldots)\cdot(2\pi)^4\delta\big(\sum_i k_i-\sum_j p_j\big) \tag{45}$$

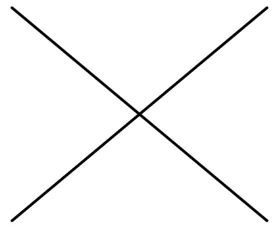

Figure 3: Fully connected diagram with one vertex. In: k_1 and k_2. Out: p_1 and p_2.

and obtain (see (41)):

$$i\mathcal{M} = \prod_i \frac{k_i^2 - m^2}{i\sqrt{Z}} \prod_j \frac{p_j^2 - m^2}{i\sqrt{Z}} \cdot \sum (\text{connected diagrams}). \tag{46}$$

Here the diagrams are interpreted with the usual momentum-space Feynman rules of correlation functions, with the simplification that there are no exponential factors or momentum integration associated with external points. With this simplification we have "external lines" instead of "external points", with a definite momentum rather than a fixed point in space.

Having demonstrated how the Fourier transforms work, our next task is to demonstrate how the factors $(k_i^2 - m^2)/i\sqrt{Z}$ and $(p_j^2 - m^2)/i\sqrt{Z}$ require us to keep only the amputated diagrams. That a diagram is "amputated" means that the legs of the diagram have been cut (and removed) as far away from the tip as possible, without cutting more than one line. (See figure p. 114 in Peskin & Schroeder.)

For concreteness we consider a general four-leg diagram (Fig. 4, left). The analysis can clearly be generalized to any number of legs. We have a central blob with diagrams relevant for scattering, in addition to diagrams on each leg. The intuition of the following is that the sum of diagrams for a leg that has been removed, transforms the bare mass m_0 into the physical mass m. Thus this part of the total diagram does not describe scattering, but rather the properties of the single particle itself. Thus if we describe the particle by its physical mass, we must only include the amputated diagrams to obtain the S matrix (Fig. 4, right).

Consider the two-point correlation function $\langle\Omega|\phi(x)\phi(y)|\Omega\rangle$, at first without time-ordering of the fields. Inserting a complete set of states

$$1 = |\Omega\rangle\langle\Omega| + \sum_\lambda \int \frac{d^3p}{(2\pi)^3} \frac{1}{2E_{\mathbf{p}}^\lambda} |\lambda_{\mathbf{p}}\rangle\langle\lambda_{\mathbf{p}}|, \tag{47}$$

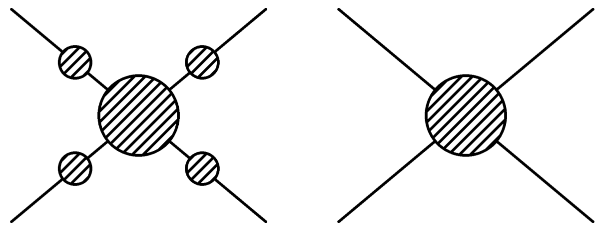

Figure 4: Left: A general four-leg Feynman diagram. Blobs represent diagrams we don't specify in detail. The small blobs contain diagrams that transform the bare mass m_0 into the physical mass m; the large blob contains diagrams relevant for scattering. Right: Amputated diagram.

and recalling (7) and (8), we obtain

$$\begin{aligned}\langle\Omega|\phi(x)\phi(y)|\Omega\rangle &= \sum_\lambda \int \frac{d^3p}{(2\pi)^3}\frac{1}{2E^\lambda_{\mathbf{p}}}\langle\Omega|\phi(x)|\lambda_{\mathbf{p}}\rangle\langle\lambda_{\mathbf{p}}|\phi(y)|\Omega\rangle \\ &= \sum_\lambda Z_\lambda \int \frac{d^3p}{(2\pi)^3}\frac{1}{2E^\lambda_{\mathbf{p}}}e^{-ip(x-y)}, \end{aligned} \tag{48}$$

with $Z_\lambda = |\langle\Omega|\phi(0)|\lambda_0\rangle|^2$ and $p^0 = E^\lambda_{\mathbf{p}}$. Introducing time-ordering, and considering the two cases $x^0 > y^0$ and $x^0 < y^0$ separately, one finds with the help of contour integration wrt. p^0 (see similar discussion of the Feynman propagator for the free Klein-Gordon field) that (48) generalizes to

$$\langle\Omega|T\phi(x)\phi(y)|\Omega\rangle = \sum_\lambda Z_\lambda \int \frac{d^4p}{(2\pi)^4}\frac{i}{p^2-m^2_\lambda+i\epsilon}e^{-ip(x-y)}. \tag{49}$$

Thus the Fourier transform of $\langle\Omega|T\phi(x)\phi(0)|\Omega\rangle$ wrt. x is

$$\int d^4x \langle\Omega|T\phi(x)\phi(0)|\Omega\rangle e^{ipx} = \sum_\lambda \frac{iZ_\lambda}{p^2-m^2_\lambda+i\epsilon}. \tag{50}$$

Setting $y = 0$ and taking the Fourier transform wrt. x amount to omitting the factors e^{-ipx} and e^{ipy} of the external points, and the integral $\int \frac{d^4p}{(2\pi)^4}$, in the momentum-space Feynman rules. Thus with this simplification of Feynman rules, (50) is the sum of all connected two-point diagrams. Eq. (50) means that for p^2 close to m^2 (where m is the physical single particle mass),

$$\int d^4x \langle\Omega|T\phi(x)\phi(0)|\Omega\rangle e^{ipx} = \frac{iZ}{p^2-m^2+i\epsilon} + \text{regular terms}. \tag{51}$$

To use (46) we need the sum of all connected diagrams. This is equal to the sum of all amputated four-leg diagrams, multiplied by four factors, the sum of all diagrams for each leg. Each of the four factors is a sum of all connected two-leg diagrams. Thus they are described by (50) or (51). Substituting into the LSZ formula (46) the four factors of the type (51) cancel the factors $(k_i^2 - m^2)/i\sqrt{Z}$ and $(p_j^2 - m^2)/i\sqrt{Z}$, and replace them by $\sqrt{Z}^4$.

For S matrix elements with $n + m$ external lines (or n particles in and m out) we therefore end up with

$$i\mathcal{M}(\mathbf{k}_1, \ldots, \mathbf{k}_m, \mathbf{p}_1, \ldots, \mathbf{p}_n) = \sqrt{Z}^{n+m} \cdot \sum(\text{connected, amputated diagrams}), \tag{52}$$

still assuming $\mathbf{k}_i \neq \mathbf{p}_j$. Here the diagrams have $n + m$ external lines. Again the diagrams are translated to expressions using a version of the momentum-space Feynman rules in which the exponential factors of external points of the corresponding correlation functions, and associated momentum integrals, are omitted. Eq. (52) with Feynman rules corresponds to (4.104) in Peskin & Schroeder, pp. 114-115.[2]

In the case with only four legs, we may argue that the diagrams not only must be connected, but fully connected. Fully connected means that all external lines are connected to all external lines. Arguing that only the fully connected diagrams matter in this case, is left as an exercise (problem set 9).

References

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[2] Although the factor $\sqrt{Z}^{n+m}$ is not included in P&S (4.104), it should be there, as they mention right after the Feynman rules ("still isn't quite correct").