# Chapter 1
# *S* and *T* Matrices. Unitarity

The typical situation of a scattering process that we deal in the subsequent is that corresponding to short-range interactions. Therefore, in the asymptotic past and future the initial and final states of particles, respectively, behave as free ones. The corresponding states are given by the direct product of monoparticle states, each of them being characterized by its three-momentum $\mathbf{p}$, spin $s$, third component of spin $\sigma$, mass $m$ and other quantum numbers (like charges) are denoted globally by $\lambda$. The corresponding state is written as

$$|\mathbf{p}, \sigma, m, s, \lambda\rangle, \tag{1.1}$$

with $\sigma = -s, -s+1, \ldots, s-1, s$. These states have the relativistic invariant normalization

$$\langle \mathbf{p}', \sigma', m', s', \lambda' | \mathbf{p}, \sigma, m, s, \lambda\rangle = \delta_{s's}\delta_{\sigma'\sigma}\delta_{\lambda'\lambda}(2\pi)^3 2p^0\delta(\mathbf{p}' - \mathbf{p}), \tag{1.2}$$

where $p^0 = \sqrt{m^2 + \mathbf{p}^2}$ is the on-shell energy.

The probability amplitude for an initial state $|i\rangle$ at time $t \to -\infty$ to evolve into a final state $|f\rangle$ at time $t \to +\infty$ is given by the matrix elements of a unitary operator $S$ denoted as the $S$ matrix [1],

$$SS^\dagger = S^\dagger S = I. \tag{1.3}$$

Its matrix elements $S_{fi}$ correspond to

$$S_{fi} = \langle f|S|i\rangle. \tag{1.4}$$

Because of the space-time homogeneity these matrix elements are always accompanied by an energy-momentum Dirac delta function, $(2\pi)^4\delta^{(4)}(p_f - p_i)$, where $p_i$ and $p_f$ are the initial an final four-momenta, in order. In linear relations a Dirac delta function of total energy and momentum conservation factors out while, in nonlinear



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relations (like unitarity), others remain, multiplying $S$-matrix elements of clusters of particles which control the momentum loops in the processes. We do not always show explicitly the cancelation of the total energy-momentum Dirac delta functions, though the context makes it clear.

In the Dirac or interacting picture of Quantum Field Theory (QFT), with $\mathcal{L}_{\text{int}}$ the interacting Lagrangian, the $S$-matrix is given by the evaluation of the matrix elements

$$S_{fi} = \frac{\langle f|e^{i\int d^4x\mathcal{L}_{\text{int}}}|i\rangle}{\langle 0|e^{i\int d^4x\mathcal{L}_{\text{int}}}|0\rangle}, \tag{1.5}$$

with $|0\rangle$ the free state without any particle (or $0_{\text{th}}$-order perturbative vacuum). In the previous equation $U(+\infty, -\infty) = \exp i\int d^4x\mathcal{L}_{\text{int}}(x)$ is the evolution operator in the interacting picture from/to asymptotic times and, therefore, $S_{fi}$ is its matrix element between the pertinent final and initial states. The denominator is a normalization factor that removes the disconnected contributions without involving any external particle.

Associated with the $S$ matrix we also have the $T$ matrix, which at least requires the presence of one interaction. Its relation with the $S$ matrix is

$$S = I + iT. \tag{1.6}$$

In terms of the $T$ matrix the unitarity relation of Eq. (1.3) reads

$$T - T^\dagger = iTT^\dagger \tag{1.7}$$

$$= iT^\dagger T, \tag{1.8}$$

by using either the first term or the second one from left to right in Eq. (1.3), respectively. By including a resolution of the identity between the product of two $T$ matrices, we have for the matrix elements

$$\begin{aligned}\langle f|T|i\rangle - \langle f|T^\dagger|i\rangle = i\sum\int &\left[(2\pi)^4\delta^{(4)}(p_f - \sum_{i=1}^n q_i)\prod_{i=1}^n \frac{d^3q_i}{(2\pi)^3 2q_i^0}\right] \\ &\times\langle f|T^\dagger|\mathbf{q}_1, \sigma_1, m_1, s_1, \lambda_1; \ldots; \mathbf{q}_n, \sigma_n, m_n, \lambda_n\rangle \\ &\times\langle \mathbf{q}_1, \sigma_1, m_1, \lambda_1; \ldots; \mathbf{q}_n, \sigma_n, m_n, \lambda_n|T|i\rangle,\end{aligned} \tag{1.9}$$

where the total energy-momentum conservation, $p_f = p_i$, should be understood. We also have the similar term in the right-hand side (rhs) but with $T^\dagger$ and $T$ exchanged. The sum extends over all the possible intermediate states allowed by the appropriate quantum numbers and with thresholds below the total center-of-mass (CM) energy $\sqrt{p_f^2}$ (otherwise the intermediate Dirac delta function would vanish).

The basic content of Hermitian unitarity (chapter 4.6 of Ref. [2]) is precisely to show that the matrix elements of $T^\dagger$ are also given by the same analytical function as those of $T$ itself but with a slightly negative imaginary part in the total energy (or partial ones for subprocesses) along the real axis, instead of the slightly positive imaginary part used for the matrix elements of $T$ in Eq. (1.9). Therefore, the unitarity relation of Eq. (1.9) gives rise to the presence of the right-hand cut (RHC) or unitarity cut in the scattering amplitudes for the total energy real and larger than the smallest threshold, typically a two-body state. It also embraces other singularities like pole ones, while its iteration from the simplest singularities (pole and normal thresholds) generates more complicated ones such as the anomalous thresholds (sections 4.10 and 4.11 of Ref. [2]).

The factor between square brackets on the rhs of Eq. (1.9) is the differential phase space of the intermediate state $|\mathbf{q}_1, \sigma_1, m_1, \lambda_1; \ldots; \mathbf{q}_n, \sigma_n, m_n, \lambda_n\rangle$. We designate it by $dQ$ and it is worth writing it isolatedly, given its importance in collision theory,

$$\int dQ = \int (2\pi)^4 \delta^{(4)}(p_f - \sum_{i=1}^{n} q_i) \prod_{i=1}^{n} \frac{d^3 q_i}{(2\pi)^3 2 q_i^0}. \tag{1.10}$$

Notice that the phase factor is Lorentz invariant.

In general the final and the initial states do not need to contain the same particles, even in nonrelativistic scattering. The latter is a valid limit as long as the three momenta of the particles involved are much smaller than their masses. This condition is required because then the Compton wavelength is much smaller than the De Broglie wavelength, $\hbar/mc \ll \hbar/|\mathbf{p}|$, and we can consider that measuring position is meaningful within good accuracy [3].

Given an initial state of two particles with four-momenta $p_1$ and $p_2$, its cross section to a final state $|f\rangle$, denoted by $\sigma_{fi}$, is defined as the number of particles scattered per unit time divided by the incident flux $\phi_0$. The latter division is necessary because the number of collisions rises in a given experiment as the number of incident particles. In our normalization, Eq. (1.2), we have the following expression for $\sigma_{fi}$ in the CM,

$$\sigma_{fi} = \frac{1}{4|\mathbf{p}_1|\sqrt{s}} \int dQ_f \, |\langle f|T|\mathbf{p}_1, \sigma_1, m_1, s_1, \lambda_1; \mathbf{p}_2, \sigma_2, m_2, s_2, \lambda_2\rangle|^2 \,, \tag{1.11}$$

where $s$ is the Lorentz invariant $s = (p_1 + p_2)^2$.

For pedagogical reasons we explain how the different factors arise in the previous formula. First, we take the modulus squared of the matrix element of the $T$ matrix, from where a factor $[(2\pi)^4 \delta^{(4)}(p_f - p_i)]^2$ arises. One of this Dirac delta function is included in the phase space $dQ_f$, while the other gives rise to the diverging factor $V\mathcal{T}$, with $V$ the volume of space and $\mathcal{T}$ the interaction time. The latter cancels because we have to divide by the time of interaction $\mathcal{T}$, since we are seeking the transition probability per unit time. On the other hand, the number of states corresponding to the normalization of monoparticle states, Eq. (1.2), is $V2p^0$. Therefore, the flux factor $\phi_0 = 4p_1^0 p_2^0 v_{\text{rel}} V$, which takes into account that there are $4p_1^0 p_2^0 V^2$ interacting particles with a relative velocity $v_{\text{rel}}$. The latter is given in the CM ($\mathbf{p}_1 + \mathbf{p}_2 = 0$) by

$$v_{\text{rel}} = \left| \frac{\mathbf{p}_1}{p_1^0} - \frac{\mathbf{p}_2}{p_2^0} \right| = \frac{|\mathbf{p}_1|(p_1^0 + p_2^0)}{p_1^0 p_2^0}. \tag{1.12}$$

Notice that in the CM $p_1^0 + p_2^0 = \sqrt{s}$. As a result the factors of $V$ cancel in the calculation of $\sigma_{fi}$ and we are left with Eq. (1.11). In particular, the total cross section from the initial state, $\sigma_i$, is given by the sum over all the possible final sates. From Eq. (1.11) we then have

$$\sigma_i = \frac{1}{4|\mathbf{p}_1|\sqrt{s}} \sum_f \int dQ_f \, |\langle f|T|\mathbf{p}_1, \sigma_1, m_1, s_1, \lambda_1; \mathbf{p}_2, \sigma_2, m_2, s_2, \lambda_2\rangle|^2 . \tag{1.13}$$

Needless to say that the sum over $f$ could also involve continuous variables and then instead of a discrete sum (as symbolically indicated in the previous equation) one would have to perform the corresponding integrals.

In the following, for brevity in the notation, we designate the monoparticle states by $|\mathbf{p}_1\sigma_1\lambda_1\rangle$, omitting some labels that might be inferred from the information given.

We can relate the total cross section $\sigma_i$ with the imaginary part of the forward $T$-matrix element $T_{ii}$ by taking $|f\rangle = |i\rangle$ in the unitarity relation of Eq. (1.9). We then have

$$\Im T_{ii} = \frac{1}{2} \sum_f \int dQ_f |T_{fi}|^2 = 2|\mathbf{p}_1|\sqrt{s}\, \sigma_i . \tag{1.14}$$

This result is usually referred as the optical theorem.

Had we taken instead the other order $TT^\dagger$ in the unitarity relation then we have

$$\Im T_{ii} = \frac{1}{2} \sum_f \int dQ_f |T_{if}|^2. \tag{1.15}$$

Comparing with Eq. (1.14) we then have the reciprocity relation

$$\sum_f \int dQ_f |T_{fi}|^2 = \sum_f \int dQ_f |T_{if}|^2. \tag{1.16}$$

As a consequence one could derive the important Boltzmann $H$-theorem in statistical mechanics (chapter 3.6. of Ref. [4]). Let $P_i$ be the probability distribution of having a state $i$ in an infinitesimal phase-space volume around this state, then its variation in time is governed by the balance of states $f$ ending in $i$ and the evolution from $i$ to any other state $f$. Thus,

$$\frac{dP_i}{dt} = \sum_f \int dQ_f |T_{if}|^2 P_f - P_i \sum_f \int dQ_f |T_{fi}|^2. \tag{1.17}$$

By summing over all initial state $i$ it is clear that

$$\sum_i \int \frac{d^4 p_i}{(2\pi)^4} \int dQ_i \frac{dP_i}{dt} = 0, \tag{1.18}$$

where the first integration involves the total four-momentum of the state $i$, to remove the extra factor of $(2\pi)^4 \delta^{(4)}(p_i - \sum_j q_j)$ included in $dQ_i$ in the next integral symbol. Physically it represents to allow all possible CM motion, since we are summing over all state $i$.

In order to simplify the derivation of the Boltzmann theorem, let us take the discretized version of the probability distribution function. Then, the entropy is defined by $S = -\sum_i P_i \log P_i$ (there would be just a constant of difference with respect to taking the continuum distribution probability function) and its derivative with respect to time is

$$\frac{dS}{dt} = -\sum_i (\log P_i + 1) \frac{dP_i}{dt} = -\sum_i \frac{dP_i}{dt} - \sum_i \frac{dP_i}{dt} \log P_i. \tag{1.19}$$

The term $-\sum_i dP_i/dt = 0$ because of Eq. (1.18), while for the last term we use the balance Eq. (1.17)

$$\frac{dS}{dt} = -\sum_i \frac{dP_i}{dt} \log P_i = -\sum_{i,j} \log P_i \left( P_j |T_{ij}^D|^2 - P_i |T_{ji}^D|^2 \right), \tag{1.20}$$

with the superscript $D$ indicating that the modulus squared of the matrix element contains the factor $(2\pi)^4 \delta^{(4)}(p_j - p_i)$, which is symmetric under $i \leftrightarrow j$. Exchanging the indices $i$ and $j$ in the last term of Eq. (1.20), we are left with

$$\frac{dS}{dt} = \sum_{i,j} |T_{ij}^D|^2 P_j \log \frac{P_j}{P_i}. \tag{1.21}$$

Now one makes use of the inequality for any two positive quantities $P_i$ and $P_j$, $P_j \log(P_j/P_i) \geq P_j - P_i$.[1] Then, the rhs of Eq. (1.21) is larger or equal than

[1]For $P_j \geq P_i$ this is clear because then $\log P_j/P_i \geq 1$. In the range $P_j \in [0, P_i]$ the difference $P_j \log(P_j/P_i) - P_j + P_i$ is $\geq 0$, because it has a negative derivative with respect to $P_j$ and it is zero at $P_j = P_i$ (it is $P_i$ for $P_j = 0$).

$\sum_{i,j} |T_{ij}^D|^2 (P_j - P_i)$. Exchanging again the indices $i$ and $j$ in the last term we are then left with the inequality

$$\frac{dS}{dt} \geq \sum_{i,j} P_j \left( |T_{ij}^D|^2 - |T_{ji}^D|^2 \right) = 0, \tag{1.22}$$

where in the last step we have taken into account the unitarity implication of Eq. (1.18).