S matrix and cross section

We have arrived to the point of the course that we are going to discuss how to compute experimentally observable collision cross sections within the apparatus of quantum field theory.

S matrix

We consider a collision of two particles. We assume that the initial state particles interact with each other only shortly before the collision and the final state particles interact with each other only shortly after the collision. Except the short interval of time the particle are be treated as non-interacting.

Definition and general properties

- The transition probability $P(i \to f)$ from the initial state $|i\rangle$ to the final one $|f\rangle$ is

$$P(i \to f) \equiv \left|\langle f|\hat{S}|i\rangle\right|^2. \tag{1}$$

  where $\hat{S}$ is the evolution operator from $-\infty$ to ∞ that is

$$\hat{S} \equiv \lim_{t\to\infty} \hat{U}(t, -t), \tag{2}$$

  where $\hat{U}(t_f, t_i)$ is the evolution operator discussed at the previous lecture.

- As we know from the previous lecture, in the interaction picture we have

$$\hat{S}_{\rm int} = \mathbb{1} - i\int_{-\infty}^{\infty} dt\, \hat{H}^I_{\rm int}(t) + \frac{(-i)^2}{2!}\int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} dt_2\, T\hat{H}^I_{\rm int}(t_1)\, \hat{H}^I_{\rm int}(t_2) + \dots \tag{3}$$

- We are interested not in the operator $\hat{S}$ but in its matrix elements

$$S_{fi} \equiv \langle f|\hat{S}|i\rangle \tag{4}$$

  which can be computed in any picture, as a unitary transformation does not change matrix elements.

- If $\hat{\mathcal{U}}$ is a unitary operator ($\hat{\mathcal{U}}\hat{\mathcal{U}}^\dagger = \hat{\mathcal{U}}^\dagger\hat{\mathcal{U}} = \mathbb{1}$) which transforms the states and the operator $\hat{S}$

$$|i'\rangle = \hat{\mathcal{U}}|i\rangle, \qquad |f'\rangle = \hat{\mathcal{U}}|f\rangle, \qquad \hat{S}' \longrightarrow \hat{U}\hat{S}\hat{U}^\dagger,$$
$$\langle i'| = \langle i|\hat{\mathcal{U}}^\dagger, \qquad \langle f'| = \langle f|\hat{\mathcal{U}}^\dagger,$$

  we have

$$\langle f'|\hat{S}'|i'\rangle = \langle f|\hat{\mathcal{U}}^\dagger\hat{\mathcal{U}}\hat{S}\hat{U}^\dagger\hat{\mathcal{U}}|i\rangle = \langle f|\hat{S}|i\rangle. \tag{5}$$

- The matrix S is unitary as the transition probability summed over all final states equals unity. Consequently,

$$\sum_f |S_{fi}|^2 = \sum_f S^*_{fi}S_{fi} = \sum_f (S^\dagger)_{if}S_{fi} = 1, \tag{6}$$

  where we sum over the complete set of final states, and $\hat{S}^\dagger\hat{S} = \mathbb{1}$. Strictly speaking the condition of unitarity is somewhat stronger $\sum_f (S^\dagger)_{if}S_{fj} = \sum_f S^*_{fi}S_{fj} = \delta^{ij}$.

Reaction operator $\hat{T}$ and optical theorem

- The reaction operator $\hat{T}$ is defined as
$$\hat{S} = \mathbb{1} + i\hat{T}. \tag{7}$$
- If there is no interaction $\hat{T} = 0$ and $\hat{S} = \mathbb{1}$. The unit operator contributes to S_{ii} but $S_{fi} = iT_{fi}$ if $f \neq i$. The states are assumed to be mutually orthogonal.
- Since $\hat{S}^\dagger \hat{S} = 1$, we have $\hat{T}^\dagger \hat{T} = -i(\hat{T} - \hat{T}^\dagger)$ which sandwiched between $\langle i|$ and $|i\rangle$ gives
$$\langle i|\hat{T}^\dagger \hat{T}|i\rangle = -i\big(\langle i|\hat{T}|i\rangle - \langle i|\hat{T}^\dagger|i\rangle\big). \tag{8}$$
Introducing the complete set of states $|f\rangle$ which satisfies the completeness condition
$$\sum_f |f\rangle\langle f| = 1 \tag{9}$$
and observing that
$$\langle i|\hat{T}|i\rangle - \langle i|\hat{T}^\dagger|i\rangle = 2i\mathrm{Im}\langle i|\hat{T}|i\rangle, \tag{10}$$
one finds the relation
$$\sum_f \langle i|\hat{T}^\dagger|f\rangle\langle f|\hat{T}|i\rangle = 2\mathrm{Im}\langle i|\hat{T}|i\rangle, \tag{11}$$
which can be rewritten as
$$\sum_f |T_{fi}|^2 = 2\mathrm{Im}T_{ii}. \tag{12}$$
It is known as the optical theorem. The quantity T_{ii} is the amplitude of zero-degree scattering where the initial and final states coincide. The sum $\sum_f |T_{fi}|^2$ is proportional to the total cross section.

Cross section

- The transition amplitude T_{fi} vanishes if the initial four-momentum P_i differs for the final four-momentum P_f. So, we can write
$$T_{fi} = (2\pi)^4 \delta^{(4)}(P_i - P_f)\, M_{fi}, \tag{13}$$
where the new amplitude M_{fi} is introduced.
- Since we are ultimately interested in the transition probability $|T_{fi}|^2$ we have
$$|T_{fi}|^2 = \big[(2\pi)^4 \delta^{(4)}(P_f - P_i)\big]^2 |M_{fi}|^2. \tag{14}$$
We encounter here a mathematical difficulty. The Dirac delta gives a meaningful expression if integrated over its argument. However,
$$\int \frac{d^4P_i}{(2\pi)^4} \big[(2\pi)^4 \delta^{(4)}(P_f - P_i)\big]^2 = (2\pi)^4 \delta^{(4)}(0) \tag{15}$$
is of unclear meaning.
- The Dirac delta $\delta^{(4)}(p)$ can be expressed as
$$(2\pi)^4 \delta^{(4)}(p) = \int d^4x\, e^{ipx}. \tag{16}$$
If $p = 0$ we have
$$(2\pi)^4 \delta^{(4)}(p = 0) = \int d^4x = V\mathcal{T}, \tag{17}$$
where V is the volume of the system under study and $\mathcal{T}$ is the time interval in which the reaction $i \to f$ is considered.

- Instead of (14) we write

$$|T_{fi}|^2 = (2\pi)^4 \delta^{(4)}(P_f - P_i)\, V\mathcal{T}\, |M_{fi}|^2. \tag{18}$$

- Another method to resolve the difficulty is to discretize the momentum space.

- We consider a collision of two particles with four-momenta $p_1 = (E_1, \mathbf{p}_1)$ i $p_2 = (E_2, \mathbf{p}_2)$. In the final state there are $n \geqslant 2$ particles with four-momenta $p'_1 = (E'_1, \mathbf{p}'_1),\ p'_2 = (E'_2, \mathbf{p}'_2),\ \ldots p'_n = (E'_n, \mathbf{p}'_n)$. The cross section is

$$d\sigma = \frac{1}{J}\frac{|T_{fi}|^2}{\mathcal{T}}\frac{V d^3p'_1}{(2\pi)^3}\frac{V d^3p'_2}{(2\pi)^3}\cdots\frac{V d^3p'_n}{(2\pi)^3}, \tag{19}$$

where J is the flux of colliding particles

$$J = \frac{|\mathbf{v}_1 - \mathbf{v}_2|}{V}, \tag{20}$$

with $\mathbf{v}_1||\mathbf{v}_2$ (in general $J = \frac{1}{V}\sqrt{(\mathbf{v}_1 - \mathbf{v}_2)^2 - (\mathbf{v}_1 \times \mathbf{v}_2)^2}$) and $\frac{V d^3p'_i}{(2\pi)^3}$ is the phase-space element of the $i-$th final state particle.

- Substituting the expressions (18, 20) into the definition (19) we obatin

$$d\sigma = \frac{V^2}{|\mathbf{v}_1 - \mathbf{v}_2|}(2\pi)^4\delta^{(4)}(P_f - P_i)\,|M_{fi}|^2\frac{V d^3p'_1}{(2\pi)^3}\frac{V d^3p'_2}{(2\pi)^3}\cdots\frac{V d^3p'_n}{(2\pi)^3}, \tag{21}$$

where $P_i = p_1 + p_2$ and $P_f = p'_1 + p'_2 + \cdots + p'_n$. As we will see, the normalization volume V disappears in final cross-section formulas.

Lorentz invariant cross-section formula

- Since a cross section is interpreted as an area perpendicular to the collision axis, it is expected to be invariant under Lorentz boosts along collision axis. We are going to rewrite the formula (21) in the Lorentz invariant form.

- We note that if $\mathbf{v}_1||\mathbf{v}_2$, we have

$$E_1E_2|\mathbf{v}_1 - \mathbf{v}_2| = \sqrt{(p_1\cdot p_2)^2 - m_1^2m_2^2}, \tag{22}$$

where $(p_1 \cdot p_2)$ is the scalar product of the four-momenta p_1 and p_2. So, $E_1E_2|\mathbf{v}_1 - \mathbf{v}_2|$ is the Lorentz scalar.

Exercise: Prove the equality (22).

- We introduce the Lorentz invariant phase-space element

$$\frac{d^3p}{E} = 2d^4p\,\Theta(p_0)\,\delta(p^2 - m^2). \tag{23}$$

The right hand side of Eq. (23) shows that it is indeed Lorentz invariant.

Exercise: Prove the equality (23).

- Using the quantities (22, 23), the cross section (21) becomes

$$d\sigma = \frac{(2\pi)^4\delta^{(4)}(P_f - P_i)}{\sqrt{(p_1\cdot p_2)^2 - (m_1m_2)^2}}\,|\mathcal{M}_{fi}|^2\frac{d^3p'_1}{(2\pi)^3E'_1}\frac{d^3p'_2}{(2\pi)^3E'_2}\cdots\frac{d^3p'_n}{(2\pi)^3E'_n}, \tag{24}$$

where the amplitude $\mathcal{M}_{fi}$ is

$$\mathcal{M}_{fi} \equiv \sqrt{V^{n+2}E_1E_2E'_1E'_2\ldots E'_n}\; M_{fi} \tag{25}$$

and it is related to T_{fi} as

$$T_{fi} = (2\pi)^4\delta^{(4)}(P_i - P_f)\,\frac{\mathcal{M}_{fi}}{\sqrt{V^{n+2}E_1E_2E'_1E'_2\ldots E'_n}}. \tag{26}$$

The cross section (24) is Lorentz invariant if the amplitude $\mathcal{M}_{fi}$ is invariant.

Interaction with infinitely heavy target

- When a target is much heavier than a projectile the latter is often treated as an infinitely heavy object at rest. Then, the momentum is not conserved in such collision even so the energy is conserved. In such a case instead of the matrix M_{fi} given by the formula (13) one uses the matrix V_{fi} related to T_{fi} as

$$T_{fi} = 2\pi\, \delta(E_i - E_f)\, V_{fi}, \tag{27}$$

and

$$|T_{fi}|^2 = 2\pi\, \delta(E_i - E_f)\, \mathcal{T}\, |V_{fi}|^2. \tag{28}$$

- The cross-section formula (21) changes into

$$d\sigma = \frac{V}{|\mathbf{v}|}\, 2\pi\, \delta(E_i - E_f)\, |V_{fi}|^2 \frac{V d^3p_1'}{(2\pi)^3} \frac{V d^3p_2'}{(2\pi)^3} \dots \frac{V d^3p_n'}{(2\pi)^3}, \tag{29}$$

where $\mathbf{v}$ is the projectile velocity.

Cross section averaged over spin

- We often deal with particles with spin which, however, is not measured. The particles are usually not polarized that is all spin states are equally probable. Then, one uses the cross section which is summed over spin states of initial particles and averaged over spin states of final state particles which is

$$d\bar{\sigma} = \frac{1}{(2S_1+1)(2S_2+1)} \sum_{s_1,s_2} \sum_{s_1',s_2',\dots} d\sigma, \tag{30}$$

where S_1 and S_2 are spins of initial state particles, s_1 and s_2 label the spin states of initial particles and $s_1', s_2', \dots$ label spin states of final state particles.

Binary processes

- A process is called <u>binary</u> if there two particles in the initial state and two particles in the final state.
- The particles' four-momenta and masses are denoted as p_1, p_2 and m_1, m_2 for the initial state and p_1', p_2' and m_1', m_2' for the final state. Due to the energy-momentum conservation we have $p_1 + p_2 = p_1' + p_2'$.
- The Lorentz invariant cross section of the binary process is

$$d\sigma = \frac{(2\pi)^4 \delta^{(4)}(P_f - P_i)}{\sqrt{(p_1 \cdot p_2)^2 - (m_1 m_2)^2}}\, |\mathcal{M}_{fi}|^2 \frac{d^3p_1'}{(2\pi)^3 E_1'} \frac{d^3p_2'}{(2\pi)^3 E_2'}. \tag{31}$$

- The process $p_1, p_2 \to p_1', p_2'$ is can be characterized by two out of three Lorentz invariant Mandelstam variables

$$s \equiv (p_1 + p_2)^2 = (p_1' + p_2')^2, \tag{32}$$

$$t \equiv (p_1 - p_1')^2 = (p_2' - p_2)^2, \tag{33}$$

$$u \equiv (p_1 - p_2')^2 = (p_1' - p_2)^2, \tag{34}$$

which obey the constraint

$$s + t + u = m_1^2 + m_2^2 + {m'}_1^2 + {m'}_2^2. \tag{35}$$

The constraint follows form the energy-momentum conservation.

<u>Exercise</u>: Prove the relation (35).

- We are going to express the cross section (31) through the invariants s, t, u. Taking the integral over $\mathbf{p}_2'$ we eliminate the delta function of momentum conservation. Using

$$d^3 p_1' = d\Omega\, d|\mathbf{p}_1'| {\mathbf{p}_1'}^2, \tag{36}$$

where $d\Omega$ is the element of the scattering solid angle of particle with $\mathbf{p}_1'$. The integral over $|\mathbf{p'}_1|$ removes the delta function of energy conservation. It can be easily taken in the center-of-mass frame where

$$\mathbf{p} \equiv \mathbf{p}_1 = -\mathbf{p}_2, \qquad \mathbf{p}' \equiv \mathbf{p}_1' = -\mathbf{p}_2'. \tag{37}$$

- Since the cross section (31) is Lorentz invariant it can be computed in any reference frame.
- In the center of mass one finds

$$\int d|\mathbf{p}'|\, \delta\Big(E_i - \sqrt{\mathbf{p}'^2 + {m'}_1^2} - \sqrt{\mathbf{p}'^2 + {m'}_1^2}\,\Big) = \frac{1}{\frac{|\mathbf{p}'|}{E_1'} + \frac{|\mathbf{p}'|}{E_2'}} = \frac{E_1' E_2'}{|\mathbf{p}'|(E_1' + E_2')}, \tag{38}$$

and the cross section (31) equals

$$\frac{d\sigma}{d\Omega} = \frac{|\mathcal{M}_{fi}|^2}{\sqrt{(p_1\cdot p_2)^2 - m_1^2 m_2^2}}\, \frac{|\mathbf{p}'|}{(2\pi)^2 (E_1' + E_2')}. \tag{39}$$

The solid angle $d\Omega$ is $d\Omega = \sin\theta d\theta\, d\phi$ where θ is the scattering angle that is the angle between $\mathbf{p}'$ and $\mathbf{p}$, and ϕ is the azimuthal angle.

- The scattering angle is related to the invariant t as

$$t = (E_1 - E_1')^2 - (\mathbf{p} - \mathbf{p}')^2 = m_1^2 + {m'}_1^2 - 2E_1 E_1' + 2|\mathbf{p}||\mathbf{p}'|\cos\theta. \tag{40}$$

- Since E_1, E_2', $|\mathbf{p}|$, $|\mathbf{p}'|$ are all independent of the scattering angle one finds

$$dt = 2|\mathbf{p}||\mathbf{p}'|\, d(\cos\theta) = -2|\mathbf{p}||\mathbf{p}'|\, \sin\theta d\theta, \tag{41}$$

which gives

$$\frac{d\sigma}{dt\, d\phi} = -\frac{1}{8\pi^2} \frac{|\mathcal{M}_{fi}|^2}{(p_1\cdot p_2)^2 - m_1^2 m_2^2}, \tag{42}$$

where we have taken into account that

$$|\mathbf{p}|(E_1' + E_2') = |\mathbf{p}|(E_1 + E_2) = \sqrt{(p_1\cdot p_2)^2 - m_1^2 m_2^2}. \tag{43}$$

- Since

$$(p_1\cdot p_2)^2 - m_1^2 m_2^2 = \frac{1}{4}\left(s^2 - 2s(m_1^2 + m_2^2) + (m_1^2 - m_2^2)^2\right), \tag{44}$$

the cross section (42) can be rewritten using the invariant s, but the formula is not simpler.

- The dependence of the cross section (42) on the azimuthal angle ϕ is absent if we deal with spinless or unpolarized particles. Then, the cross section reads

$$\frac{d\sigma}{dt} = -\frac{1}{4\pi} \frac{|\mathcal{M}_{fi}|^2}{(p_1\cdot p_2)^2 - m_1^2 m_2^2}. \tag{45}$$