Specialization report

Heinrich Heine Universität Düsseldorf
Institut für Theoretische Physik I

Presented by:
Marius Theißen
Matrn.: 2163903

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Contents

1 Introduction

Quantum field theory is a formalism that allow us to describe the interaction between elementary particles. Of great interest are observable quantities like cross-sections or decay rates, which can be established theoretically and contrasted with experimental results. Both observables can be determined from the amplitude of the corresponding process. Which are calculated by using pertubation theory. The main goal of this report is the derivation of the Gell-Mann Low formula that enables us to apply this technique.

In chapter 2 we discuss the more common Schrödinger, Heisenberg and Interaction picture. Followed up by *in* and *out* pictures to which Gell-Mann Low formula allows easy transition. These pictures are based on boundary conditions, which are motivated in chapter 2.3, imposing free motion on particles along them. We derive them from experimental and physical points of view. After deriving concrete solutions for the unitary operators associated with these new pictures, we define the scattering operator $\hat{S}$ in chapter 3. Finally resulting in the Gell-Mann Low formula.

2 Pictures in Quantum Mechanics

2.1 Schrödinger picture and Heisenberg picture

The choice of a picture always requires to establish the states but also the corresponding operators. In the Schrödinger picture the operators are time-independent but the wavefunctions are time dependent. The time evolution of a state vector is controlled by the Schrödinger equation. Let $|\Psi(t)\rangle$ denote a state vector at time t. It satisfies

$$i\hbar\frac{\partial}{\partial t}|\Psi_S(t)\rangle = \hat{H}|\Psi_S(t)\rangle, \tag{1}$$

where $\hat{H}$ is the Hamiltonian of the system. When assuming it time independent, the solution of Eq. (1) can be formally written as

$$|\Psi_S(t)\rangle = \hat{U}(t-t_0)|\Psi_S(t_0)\rangle \tag{2}$$

with $\hat{U}(t-t_0) = e^{-\frac{i}{\hbar}\hat{H}(t-t_0)}$ the time evolution operator, which satisfies the differential equation

$$i\hbar\partial_t\hat{U}(t-t_0) = \hat{H}\hat{U}(t-t_0). \tag{3}$$

Under the general assumption of the Hamiltonian being hermitian $\hat{U}(t - t_0)$ is also an unitary operator, meaning:

$$\hat{U}(t - t_0) \times \hat{U}^\dagger(t - t_0) = e^{-\frac{i}{\hbar}\hat{H}(t-t_0)}e^{\frac{i}{\hbar}\hat{H}(t-t_0)} = 1$$
$$= \hat{U}(t - t_0) \times \hat{U}^{-1}(t - t_0) \tag{4}$$

Going back to Eq. (2) we see $|\Psi_S(t_0)\rangle$ is a ket of $t = t_0$. We shall generally take $t_0 = 0$ and write

$$|\Psi_S(t)\rangle = e^{-\frac{i}{\hbar}\hat{H}t}|\Psi_H\rangle . \tag{5}$$

The state on the right-hand side has no longer time dependence. This defines the state in the Heisenberg picture.

The above two pictures differ between each other in the way of storing the time dependence. In the Schrödinger picture only the states carry such a dependence, whereas in the Heisenberg picture only operators has this possibility. To verify this statement we study the matrix element of an operator in the Schrödinger picture

$$\langle \Psi'_S(t)| \hat{A}_S |\Psi_S(t)\rangle = \langle \Psi'_H| e^{\frac{i}{\hbar}t\hat{H}}\hat{A}_S e^{-\frac{i}{\hbar}t\hat{H}} |\Psi_H\rangle , \tag{6}$$

where Eq. (5) has been used. As a consequence,

$$\hat{A}_H(t) = e^{\frac{i}{\hbar}t\hat{H}}\hat{A}_S e^{-\frac{i}{\hbar}t\hat{H}} = \hat{U}(t)^{-1}\hat{A}_S\hat{U}(t). \tag{7}$$

This new operator $\hat{A}_H(t)$ in combination with the state $|\Psi_H\rangle$ defines the Heisenberg picture. Observe that the time evolution of $\hat{A}_H(t)$ is dictated by an equation that follows from differentiating the equation above with respect to t:

$$\frac{d}{dt}\hat{A}_H(t) = \frac{i}{\hbar}\hat{H}e^{\frac{i}{\hbar}t\hat{H}}\hat{A}_S e^{-\frac{i}{\hbar}t\hat{H}} + e^{\frac{i}{\hbar}t\hat{H}}\hat{A}_S \left(-\frac{i}{\hbar}\hat{H}\right) e^{-\frac{i}{\hbar}t\hat{H}}. \tag{8}$$

Here we have used the time evolution equation (3). Hence,

$$\frac{d}{dt}\hat{A}_H(t) = \frac{i}{\hbar}\hat{U}(t)^{-1}\hat{H}\hat{A}_S\hat{U}(t) - \frac{i}{\hbar}\hat{U}(t)^{-1}\hat{A}_S\hat{H}\hat{U}(t)$$
$$= \frac{i}{\hbar}\hat{U}(t)^{-1}\hat{H}\underbrace{\hat{U}(t)\hat{U}(t)^{-1}}_{=1}\hat{A}_S\hat{U}(t) - \frac{i}{\hbar}\hat{U}(t)^{-1}\hat{A}_S\underbrace{\hat{U}(t)\hat{U}(t)^{-1}}_{=1}\hat{H}\hat{U}(t). \tag{9}$$

The inserted 1 allows us to express Eq. (9) in term of operators in the Heisenberg picture.

$$\frac{d}{dt}\hat{A}_H(t) = \frac{i}{\hbar}\hat{H}_H(t)\hat{A}_H(t) - \frac{i}{\hbar}\hat{A}_H(t)\hat{H}_H(t), \tag{10}$$

where $\hat{H}_H(t)$ is the respective Hamiltonian in the Heisenberg picture. Therefore:

$$i\frac{d}{dt}\hat{A}_H(t) = \frac{1}{\hbar}\left[\hat{A}_H(t), \hat{H}_H(t)\right]. \tag{11}$$

2.2 Interaction picture

A third picture can be introduced: the Interaction picture (sometimes called the Dirac picture). We will see very shortly that, in the Interacting picture both the states and the respective operators are time dependent. Let us suppose that the Hamiltonian in the Schrödinger picture can be splitted as follows $\hat{H} = \hat{H}_0 + \hat{V}$. Normally $\hat{H}_0$ describe the free motion of a system, whereas $\hat{V}$ represents its interaction, which could be with an external source. Although it often used in a perturbative approach, the Interaction picture does not require $\hat{V}$ to be small as compared with $\hat{H}_0$. Inserting this decomposition of $\hat{H}$ in the unitary operator introduced below Eq. (2):

$$\hat{U}(t) = e^{-\frac{i}{\hbar}t\hat{H}} = e^{-\frac{i}{\hbar}t\left(\hat{H}_0+V\right)} = e^{-\frac{i}{\hbar}t\hat{H}_0}\hat{\Omega}_I(t) \tag{12}$$

This expression helps us to establish a formula from which operators and states in the interaction picture can be defined[1]. For this, consider a matrix element $\langle\Psi_S'(t)|\,\hat{A}_S\,|\Psi_S(t)\rangle$. Taking into account Eq. (5) and (12) we find

$$\langle\Psi_S'(t)|\,\hat{A}_S\,|\Psi_S(t)\rangle = \langle\Psi_H'|\,(e^{-\frac{i}{\hbar}t\hat{H}_0}\Omega_I(t))^\dagger\hat{A}_S e^{-\frac{i}{\hbar}t\hat{H}_0}\Omega_I(t)\,|\Psi_H\rangle \tag{13a}$$

$$= \langle\Psi_H'|\,\Omega_I(t)^{-1}\hat{A}_I(t)\Omega_I(t)\,|\Psi_H\rangle. \tag{13b}$$

Here the operator in the interaction picture reads

$$\hat{A}_I(t) = e^{+\frac{i}{\hbar}t\hat{H}_0}\,\hat{A}_S e^{-\frac{i}{\hbar}t\hat{H}_0}, \tag{14}$$

whereas a corresponding state in this picture is

$$|\Psi_I(t)\rangle = \Omega_I(t)\,|\Psi_H\rangle. \tag{15}$$

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[1]By substituting Eq. (12) in Eq. (4) one can see directly that $\Omega_I(t)$ is also unitary

At the level of operators, the connection between the Interaction and the Heisenberg picture is established by inverting Eq. (7) and inserting the resulting $\hat{A}_S$ into Eq. (14). This leads to

$$\hat{A}_I(t) = e^{+\frac{i}{\hbar}t\hat{H}_0}\hat{U}(t)\hat{A}_H(t)\hat{U}(t)^{-1}e^{-\frac{i}{\hbar}t\hat{H}_0}. \tag{16a}$$

$$= e^{+\frac{i}{\hbar}t\hat{H}_0}e^{-\frac{i}{\hbar}t\hat{H}}\hat{A}_H(t)e^{\frac{i}{\hbar}t\hat{H}}e^{-\frac{i}{\hbar}t\hat{H}_0}, \tag{16b}$$

ending with

$$\hat{A}_I(t) = \hat{\Omega}_I(t)\hat{A}_H(t)\hat{\Omega}_I(t)^{-1}. \tag{17}$$

The time evolution equation for $\hat{A}_I(t)$ can be found as done for $\hat{A}_H(t)$ [see below Eq. (7)]:

$$i\hbar\frac{\partial}{\partial t}\hat{A}_I = \left[\hat{A}_I, \hat{H}_0\right]. \tag{18}$$

Furthermore, an equation for $\hat{\Omega}_I(t)$ can be determined. To this end we invert Eq. (12) and express $\hat{\Omega}_I(t) = e^{\frac{i}{\hbar}t\hat{H}_0}\hat{U}(t)$. Afterwards we differentiate with respect to times:

$$i\hbar\partial_t\hat{\Omega}_I(t) = e^{\frac{i}{\hbar}t\hat{H}_0}\left(i\hbar\partial_t\hat{U}(t)\right) - \hat{H}_0 e^{\frac{i}{\hbar}t\hat{H}_0}\hat{U}(t) \tag{19a}$$

$$= \hat{H}e^{\frac{i}{\hbar}t\hat{H}_0}\hat{U}(t) - \hat{H}_0 e^{\frac{i}{\hbar}t\hat{H}_0}\hat{U}(t), \tag{19b}$$

where Eq. (3) has been used. Using the definition of $\hat{\Omega}_I(t)$ we end up with

$$i\hbar\frac{\partial}{\partial t}\hat{\Omega}_I(t) = \hat{V}_I(t)\hat{\Omega}_I(t). \tag{20}$$

To find a well defined solution, an initial condition is needed. In Eq. (12) we see that at $t = 0$, the time evolution operator reduces to $\hat{U}(0) = 1$, and from this the following condition $\hat{\Omega}_I(0) = 1$ arises. We remark that $\hat{V}_I(t)$ in the Interaction picture as introduced above does not require $\hat{V}$ to be of any specific form but can still be applied in presence of external sources.

2.3 The *in* and *out* picture: External currents

Consider the set-up of most experiments in elementary particle and nuclear physics. Several particles approach each other from a macroscopic scale and interact in a microscopic section comparable to the Compton wavelength of the incoming particles. On this scale vacuum fluctuations are no longer negligible for the dynamic of the involved particles and make them impossible

to distinguish between each other. As a result, the products of the interaction spread up to a macroscopic distances and the distinguishability between outgoing particles is admitted. Therefore, at such asymptotically distances, the description of the incoming and outgoing multi-particle states can be approached by direct products of single-particle effectively non-interacting states.

To bring this concept into our formulation let's consider the action of a scalar field Φ with mass $m = m_0 c/\hbar$ coupled to an external source $j(\underline{x}, t)$[2]:

$$I = \int d^4x \; \mathcal{L}(\Phi, \dot{\Phi}, j) = \int d^4x \left(\frac{1}{2} \partial_\mu \Phi \partial^\mu \Phi - \frac{1}{2} m^2 \Phi^2 - \Phi j \right). \tag{21}$$

Taking the functional derivative with respect to Φ and setting it to zero, we obtain the equation of motion

$$\left(\partial^2 + m^2 \right) \Phi = j. \tag{22}$$

To proceed, we quantize our field in a box of volume V and length L. The classical field and its canonical momentum $\Pi = \partial \mathcal{L}/\partial \dot{\Phi}(\underline{x}, t) = \dot{\Phi}(\underline{x}, t)$ are then promoted to operators $\hat{\Phi}(\underline{x}, t)$ and $\hat{\Pi}(\underline{x}, t)$ in the Heisenberg picture. Satisfying the equal-time commutator:

$$\left[\hat{\Phi}(\underline{x}, t), \hat{\Pi}(\underline{x}', t) \right] = i \delta^3(\underline{x} - \underline{x}'). \tag{23}$$

We then expand the field operator as follows:

$$\hat{\Phi}(\underline{x}, t) = \sum_{\underline{k}} \hat{q}_{\underline{k}}(t) u_{\underline{k}}(\underline{x}). \tag{24}$$

The 3 dim. wave vector $\underline{k}$ for the modes is represented by $\underline{k} = \dfrac{2\pi}{L}(n_x, n_y, n_z)$ with $n_i \in \mathbb{Z}$. In this separated time and space dependency, we choose the Fourier basis for $u_{\underline{k}}(\underline{x})$

$$u_{\underline{k}}(\underline{x}) = \frac{1}{L^{3/2}} e^{i\underline{k}\cdot\underline{x}}, \tag{25}$$

where the volume L^3 provides the required normalization. We remark that $u_{\underline{k}}(\underline{x})$ constitutes an orthonormalized basis in the Hilbert space

$$\int d^3x \; u_{\underline{k}'}^*(\underline{x}) u_{\underline{k}}(\underline{x}) = \delta_{\underline{k},\underline{k}'} \tag{26}$$

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[2]From now on we will work in natural units and set $c = \hbar = 1$

$$\sum_{\underline{k}} u_{\underline{k}}^*(\underline{x}) u_{\underline{k}}(\underline{x}') = \delta^3\left(\underline{x} - \underline{x}'\right). \tag{27}$$

We now substitute Eq. (25) into the equation of motion (22) . As a consequence

$$\sum_{\underline{k}} \left[\ddot{\hat{q}}_{\underline{k}}(t) u_{\underline{k}}(\underline{x}) + \underline{k}^2 \hat{q}_{\underline{k}}(t) u_{\underline{k}}(\underline{x}) + m^2 \hat{q}_{\underline{k}}(t) u_{\underline{k}}(\underline{x}) \right] = j(\underline{x}, t). \tag{28}$$

To get an equation for $\hat{q}_{\underline{k}}(t)$ alone we need to get rid of $u_{\underline{k}}(\underline{x})$ and remove the space dependence in the current. Multiplying with $u_{\underline{k}'}^*(\underline{x})$ and integrating over the whole space we find,

$$\sum_{\underline{k}} \left[\int d^3x \; u_{\underline{k}'}^* u_{\underline{k}} \left(\ddot{\hat{q}}_{\underline{k}}(t) + \left(\underline{k}^2 + m^2\right) \hat{q}_{\underline{k}}(t) \right) \right] = \underbrace{\int d^3x \; j(\underline{x}, t) \frac{1}{L^{3/2}} e^{i\underline{k}\cdot\underline{x}}}_{=\tilde{j}(\underline{k}, t)}. \tag{29}$$

After using the orthonormality relation (26) this expression reduces to

$$\ddot{\hat{q}}_{\underline{k}}(t) + \omega_{\underline{k}}^2 \hat{q}_{\underline{k}}(t) = \tilde{j}(\underline{k}, t), \tag{30}$$

where $\omega_{\underline{k}}^2 = (\underline{k}^2 + m^2)$ is the energy of the particle in mode $\underline{k}$.

We now make the assumption that the current vanishes outside a finite time interval,

$$j(\underline{k}, t) \to 0 \text{ for } t \to \pm\infty. \tag{31}$$

As a consequence one can distinguish between early and late times. For early time Eq. (30) approaches the homogeneous differential equation. We will call its asymptotic solution by $\hat{q}_{\underline{k}}(t) \to \hat{q}_{k,in}(t)$. Explicitly,

$$\hat{q}_{\underline{k},in}(t) \approx \frac{1}{2\omega_{\underline{k}}} \left(\hat{a}_{\underline{k},in} e^{-i\omega_{\underline{k}} t} + \hat{a}_{-\underline{k},in}^\dagger e^{i\omega_{\underline{k}} t} \right), \quad t \to -\infty, \tag{32}$$

where $\hat{a}_{\underline{k},in}$ denotes the annihilation operator, whereas $\hat{a}_{\underline{k},in}^\dagger$ is the corresponding creation operator. Their commutator is

$$\left[\hat{a}_{\underline{k},in}, \hat{a}_{\underline{k}',in}^\dagger \right] = 2\omega_{\underline{k}} \delta_{\underline{k},\underline{k}'}. \tag{33}$$

At late times Eq. (30) also reduces to a homogeneous type. In this case the asymptotic solution $\hat{q}_{\underline{k}}(t) \to \hat{q}_{k,out}(t)$ reads

$$\hat{q}_{\underline{k},out}(t) \approx \frac{1}{2\omega_{\underline{k}}} \left(\hat{a}_{\underline{k},out} e^{-i\omega_{\underline{k}} t} + \hat{a}_{-\underline{k},out}^\dagger e^{i\omega_{\underline{k}} t} \right), \quad t \to +\infty. \tag{34}$$

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The solution for $\hat{q}_{\underline{k}}(t)$, at times for which $j(\underline{x}, t)$ is active, would then consist of the homogeneous solution plus a term containing the current:

$$\hat{q}_{\underline{k}}(t) = \hat{q}_{\underline{k},in}(t) + \frac{1}{\omega_{\underline{k}}} \int_{-\infty}^{t} dt' \sin\left[\omega_{\underline{k}}(t - t')\right] \tilde{j}(\underline{k}, t'), \tag{35}$$

where $\bar{j}_{\underline{k}}(\omega_{\underline{k}}) = \int_{-\infty}^{\infty} dt \tilde{j}(\underline{k}, t) e^{i\omega_{\underline{k}} t}$ is the temporal Fourier transform of the current. For late times $t \to +\infty$ the expression above approaches to

$$\hat{q}_{\underline{k},out}(t) \approx \hat{q}_{\underline{k},in}(t) + \frac{1}{\omega_{\underline{k}}} \int_{-\infty}^{\infty} dt' \sin\left[\omega_{\underline{k}}(t - t')\right] \tilde{j}(\underline{k}, t'). \tag{36}$$

After splitting the sinus function, we find

$$\hat{q}_{\underline{k},out}(t) = \hat{q}_{\underline{k},in}(t) - \frac{i}{2\omega_{\underline{k}}} e^{i\omega_{\underline{k}} t} \, \bar{j}_{\underline{k}}(-\omega_{\underline{k}}) + \frac{i}{2\omega_{\underline{k}}} e^{-i\omega_{\underline{k}} t} \, \bar{j}_{\underline{k}}(\omega_{\underline{k}}), \tag{37}$$

From this equation we can obtain the connection between creation and annihilation operators associated with the asymptotically far fields $t \to \pm\infty$. In compact notation

$$\hat{a}_{\underline{k},out} = \hat{a}_{\underline{k},in} + i\bar{j}_{\underline{k}}(\omega_{\underline{k}}), \tag{38a}$$

$$\hat{a}^{\dagger}_{\underline{k},out} = \hat{a}^{\dagger}_{\underline{k},in} - i\bar{j}_{\underline{k}}(-\omega_{\underline{k}}). \tag{38b}$$

This shows that, in the presence of an external current, the two sets of second quantization operators are not the same. Therefore we need to differ between the corresponding *in* and *out* eigenstates. Particularly, it has to be stated that the vacua also differ in this scenario.

It is important to stress, that the full solution $\hat{q}_{\underline{k}}(t)$ found in Eq. (35) has to be understood in the Heisenberg picture. From this we can proceed as shown in section **2.2**. We split the Hamiltonian as done there: $\hat{H} = \hat{H}_0 + \hat{V}$.

$$\hat{H}_0(\Phi, \Pi) = \int d^3x \left[\frac{1}{2}\hat{\Pi}^2 + \frac{1}{2}(\nabla\hat{\Phi})^2 + \frac{1}{2}m^2\hat{\Phi}^2\right], \tag{39}$$

$$\hat{V}(\Phi) = \int d^3x \, j\hat{\Phi}. \tag{40}$$

Expressing both field operators in terms of the Fourier basis given in (24), and using the orthonormality relation Eq. (26), as well as the reality condition

of the field for $\hat{q}_{-\underline{k}}(t) = \hat{q}_{\underline{k}}^{\star}(t)$ we can express the Hamiltonian as follows:

$$\hat{H}_0(q, \dot{q}) = \sum_{\underline{k}} \left\{ \frac{1}{2}\dot{\hat{q}}_{\underline{k}}^2(t) + \frac{1}{2}\omega_{\underline{k}}^2\hat{q}_{\underline{k}}^2(t) \right\}, \tag{41}$$

$$\hat{V}(q) = \sum_{\underline{k}} \tilde{j}(\underline{k}, t)\hat{q}_{\underline{k}}(t). \tag{42}$$

From this form we go to the Interaction picture. In the present context, the potential V_I appearing in Eq. (20) reads:

$$\hat{V}_I(q_I) = \sum_{\underline{k}} \tilde{j}(\underline{k}, t)\hat{q}_{\underline{k}_I}(t), \tag{43}$$

where we used Eq. (17) to transform $\hat{q}_{\underline{k}}(t)$ into the Interaction picture

$$\hat{q}_{\underline{k}_I}(t) = \hat{\Omega}_I(t)\hat{q}_{\underline{k}}(t)\hat{\Omega}_I^{-1}(t). \tag{44}$$

To have a well defined operator $\hat{\Omega}_I(t)$ we need conditions for any $\hat{\Omega}$ so that $\hat{\Omega} \to 1$ as stated for the Interaction picture in Eq. (20) which is at the moment mostly depended on the current j. The early time condition at $t = -\infty$ defines the *in* picture in reminiscence to the first asymptotic solution given in Eq (32) and it writes:

$$i\frac{\partial}{\partial t}\hat{\Omega}_{in}(t) = \hat{V}_{in}(t)\hat{\Omega}_{in}(t), \tag{45}$$

where the initial condition $\hat{\Omega}_{in}(-\infty) = 1$ has to be fulfilled. Contrary to the previous case the operator of the *out* picture will satisfy the differential equation:

$$i\frac{\partial}{\partial t}\hat{\Omega}_{out}(t) = \hat{V}_{out}(t)\hat{\Omega}_{out}(t), \tag{46}$$

with $\hat{\Omega}_{out}(+\infty) = 1$.

3 Scattering operator

3.1 Solutions for the Interaction, *in* and *out* picture

In this section we solve the differential equations for the various pictures established in section 2.2 and 2.3. We start with the Interaction picture

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depended on t' and integrate both sides of Eq. (20). For $t > 0$ its left-hand side gives:

$$\int_0^t \mathrm{d}t' i \frac{\partial}{\partial t'} \hat{\Omega}_I(t') = i \left[\hat{\Omega}_I(t) - 1 \right], \tag{47}$$

where the initial condition $\hat{\Omega}_I(0) = 1$ has been used. With this formula and the integral over the right-hand side of (20), we find an expression for $\hat{\Omega}_I(t)$.

$$\hat{\Omega}_I(t) = 1 - i \int_0^t \mathrm{d}t' \hat{V}_I(t') \hat{\Omega}_I(t'), \tag{48}$$

since the expression has an $\hat{\Omega}_I(t)$ on the other side we will go on by an iterative approach.

$$\hat{\Omega}_I(t) = 1 - i \int_0^t \mathrm{d}t' \hat{V}_I(t') \cdot \left(1 - i \int_0^{t'} \mathrm{d}t'' \hat{V}_I(t'') \hat{\Omega}_I(t'') \right)$$
$$= 1 - i \int_0^t \mathrm{d}t' \hat{V}_I(t') + i^2 \int_0^t \mathrm{d}t' \int_0^{t'} \mathrm{d}t'' \hat{V}_I(t'') \hat{\Omega}_I(t''). \tag{49}$$

The iteration increments the power of i and the number of integrals. By repeating the operation described above we can write

$$\hat{\Omega}_I(t) = \sum_{n=0}^{\infty} (-i)^n \int_0^t \mathrm{d}t_1 \int_0^{t_1} \mathrm{d}t_2 \ldots \int_0^{t_{n-1}} \mathrm{d}t_n \hat{V}_I(t_1) \cdot \ldots \cdot \hat{V}_I(t_n). \tag{50}$$

A problematic aspect of this series are the different integral limits. Each term introduces a new t_i and keeps the previous t_{i-1} as an integral variable which forces us to solve them in a strict order. To circumvent this formal aspect we will perform some additional operations. Let us consider the term from Eq. (50) containing the product of two interactions :

$$I(t) = \int_0^t \mathrm{d}t_1 \int_0^{t_1} \mathrm{d}t_2 \hat{V}_I(t_1) \hat{V}(t_2). \tag{51}$$

By developing the change of variable $t_2 \longleftrightarrow t_1$,[3] this integral can be written as

$$I(t) = \int_0^t \mathrm{d}t_2 \int_0^{t_2} \mathrm{d}t_1 \hat{V}_I(t_2) \hat{V}_I(t_1). \tag{52}$$

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[3] The Jacobian of this change of variable is the unity

We find an alternative representation of $I(t)$ by adding (51) and (52):

$$I(t) = \frac{1}{2} \int_0^t dt_1 \int_0^{t_1} dt_2 \hat{V}_I(t_1)\hat{V}_I(t_2) + \frac{1}{2} \int_0^t dt_2 \int_0^{t_2} dt_1 \hat{V}_I(t_2)\hat{V}_I(t_1). \quad (53)$$

In order to have a common integration limit t, we introduce the chronological time ordering.

$$T(\hat{V}_I(t_1), \hat{V}_I(t_2)) = \hat{V}_I(t_1) \ \hat{V}_I(t_2) \ \theta(t_1 - t_2) \ + \ \hat{V}_I(t_2) \ \hat{V}_I(t_1) \ \theta(t_2 - t_1). \quad (54)$$

The chronological time ordering sets operators depending of earlier times to the right and later to the left. The the Heaviside-Step-function is 0 for negative values of its argument and 1 when it becomes positive. By subtracting t_1 and t_2 in the argument of the step functions we are able to switch between the two terms in Eq. (53) and extending the integral limits to t, since it sets terms to zero for negative arguments. Therefore no change appears in the result of the integral by extending the limit. We used for $t_1 > t_2 \to \theta(t_1 - t_2)$ and for $t_2 > t_1 \to \theta(t_2 - t_1)$. By applying Eq. (54) at Eq. (53), we find the desired notation:

$$I(t) = \frac{1}{2} \int_0^t dt_1 \int_0^t dt_2 \hat{V}_I(t_1) \ \hat{V}_I(t_2) \ \theta(t_1 - t_2)$$
$$+ \frac{1}{2} \int_0^t dt_1 \int_0^t dt_2 \ \hat{V}_I(t_2) \ \hat{V}_I(t_1) \ \theta(t_2 - t_1),$$

$$I(t) = \frac{1}{2!} \int_0^t dt_1 \int_0^t dt_2 T(\hat{V}_I(t_1), \hat{V}_I(t_2)). \quad (55)$$

This case of two interactions is generalized to terms involving $\hat{V}(t)$ n-times in the appendix 5.A. Applying the T operator allows us to write the solution to $\hat{\Omega}_I(t)$ given in Eq. (50) in the time-ordered form:

$$\hat{\Omega}_I(t) = \frac{(-i)^n}{n!} \int_0^t dt_1 \int_0^t dt_2 \ldots \int_0^t dt_n T\left\{\hat{V}_I(t_1), \ldots, \hat{V}_I(t_n)\right\}. \quad (56)$$

Observe that this expression is a non-pertubative result, which can be written in a symbolically notation

$$\hat{\Omega}_I(t) = T\left(e^{-i \int_0^t dt' \hat{V}_I(t')}\right), \quad \text{for } t \geq 0. \quad (57)$$

To not limit the Interaction picture only to positive t values, we need a complementary expression for negative t's. Assuming $t < 0$, the integral in Eq. (47) is changed to:

$$\int_t^0 dt' i \frac{\partial}{\partial t'} \hat{\Omega}_I(t') = i \left[1 - \hat{\Omega}_I(t) \right]. \tag{58}$$

Alongside performing in the integral of the right-hand side of Eq. (20) in the new limits, we find:

$$\hat{\Omega}_I(t) = 1 + i \int_t^0 dt' \hat{V}_I(t') \hat{\Omega}_I(t'). \tag{59}$$

From this, our infinite sum expression still holds up to a different sign:

$$\hat{\Omega}_I(t) = \sum_{n=0}^{\infty} i^n \int_t^0 dt_1 \int_{t_1}^0 dt_2 \ldots \int_{t_{n-1}}^0 dt_n \hat{V}_I(t_1) \cdot \ldots \cdot \hat{V}_I(t_n). \tag{60}$$

The key difference now stands in the negativity of all t and a logical order for them would prefer later times to the right, coming closer to 0. This requires the anti-chronological time ordering:

$$\bar{T}(\hat{V}(t_1), \hat{V}(t_2)) = \hat{V}(t_2)\, \hat{V}(t_1)\, \theta(t_1 - t_2)\; +\; \hat{V}(t_1)\, \hat{V}(t_2)\, \theta(t_2 - t_1). \tag{61}$$

A generalized expression containing the product of several $\hat{V}(t)$'s is given in the appendix 5.A. Using it similar as before:

$$\hat{\Omega}_I(t) = \sum_{n=0}^{\infty} \frac{i^n}{n!} \int_t^0 dt_1 \int_t^0 dt_2 \ldots \int_t^0 dt_n \bar{T}\left\{ \hat{V}_I(t_1), \ldots, \hat{V}_I(t_n) \right\}. \tag{62}$$

As a consequence, we obtain a second expression:

$$\hat{\Omega}_I(t) = \bar{T}\left(e^{i \int_t^0 dt' \hat{V}_I(t')} \right), \quad \text{for } t < 0. \tag{63}$$

A notation for $\hat{\Omega}_I(t)$ without specifying the values of t can be derived by using Heaviside-Step-functions:

$$\hat{\Omega}_I(t) = T\left(e^{-i \int_0^t dt' \hat{V}_I(t')} \right) \theta(t) + \bar{T}\left(e^{+i \int_t^0 dt' \hat{V}_I(t')} \right) \theta(-t). \tag{64}$$

For the *in* picture we proceed in an almost identical fashion to the Interaction picture for $t > 0$. Only the lower boundary in the integral is changed

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to $-\infty$ as it is the asymptotic condition of this picture. This resolves the need for a two term solution. After resumation, we obtain:

$$\hat{\Omega}_{in}(t) = T\left(e^{-i\int_{-\infty}^{t} dt' \hat{V}_{in}(t')}\right). \tag{65}$$

The *out* picture on the other hand follows the derivation of the expression for $t < 0$. We start at Eq. (58) with ∞ instate of 0. Here we argue t being smaller then ∞ needs one change of sign like before and anti-chronological ordering $\bar{T}$ introduced in Eq. (61), since t only coming closer to the limit as it runs.

$$\hat{\Omega}_{out}(t) = \sum_{n=0}^{\infty} \frac{(i)^n}{n!} \int_{t}^{\infty} dt_1 \int_{t}^{\infty} dt_2 \ldots \int_{t}^{\infty} dt_n \bar{T}\left\{\hat{V}_{out}(t_1), \ldots, \hat{V}_{out}(t_n)\right\}. \tag{66}$$

Performing a flip in the integral limits we conclude:

$$\hat{\Omega}_{out}(t) = \bar{T}\left(e^{-i\int_{\infty}^{t} dt' \hat{V}_{in}(t')}\right). \tag{67}$$

3.2 Representation of the Scattering operator

In section 2.3 we saw that the creation and annihilation operators associated with the *in* and *out* pictures are related between each other in Eq. (38) via the external current. We wish to establish how this connection manifests at the level of the corresponding scattering states. To this end, we particularize Eq. (15) to the case in which the initial condition is taken at $t \to \pm\infty$. If the initial condition is $t \to -\infty$, we have

$$|\Psi_{in}(t)\rangle = \hat{\Omega}_{in}(t) |\Psi_H\rangle. \tag{68}$$

Likewise for the *out* picture we write:

$$|\Psi_{out}(t)\rangle = \hat{\Omega}_{out}(t) |\Psi_H\rangle. \tag{69}$$

Combining both Eq. (68) and Eq. (69) we find

$$|\Psi_{in}(t)\rangle = \hat{\Omega}_{in}(t)\hat{\Omega}_{out}^{-1}(t) |\Psi_{out}(t)\rangle. \tag{70}$$

The product of $\hat{\Omega}$'s defines the scattering operator $\hat{S}$:

$$\hat{S} = \hat{\Omega}_{in}(t)\hat{\Omega}_{out}^{-1}(t). \tag{71}$$

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We will verify explicitly that Eq. (71) is time independent. For this we take the partial derivative of $\hat{S}$ with respect to t. This operation leads to

$$i\partial_t \left(\hat{\Omega}_{in}(t)\hat{\Omega}_{out}^{-1}(t) \right) = i\dot{\hat{\Omega}}_{in}(t)\hat{\Omega}_{out}^{-1}(t) + i\hat{\Omega}_{in}(t)\dot{\hat{\Omega}}_{out}^{-1}(t)$$
$$= \hat{V}_{in}(t)\hat{\Omega}_{in}(t)\hat{\Omega}_{out}^{-1}(t) + i\hat{\Omega}_{in}(t)\dot{\hat{\Omega}}_{out}^{-1}(t). \tag{72}$$

In the first term of the second line we have used Eq. (45). The evaluation of $\dot{\hat{\Omega}}_{out}^{-1}(t)$ requires some additional steps. We start by differentiating the identity $\hat{\Omega}_{out}(t)\hat{\Omega}_{out}^{-1}(t) = 1$. We then find the relation

$$i\hat{\Omega}_{out}(t)\dot{\hat{\Omega}}_{out}^{-1}(t) = -i\dot{\hat{\Omega}}_{out}(t)\hat{\Omega}_{out}^{-1}(t) \tag{73}$$

Afterwards, we multiply the left by $\hat{\Omega}_{out}(t)$ and use Eq. (46) in the right-hand side. As a consequence,

$$i\dot{\hat{\Omega}}_{out}^{-1}(t) = -\hat{\Omega}_{out}^{-1}(t)\hat{V}_{out}(t). \tag{74}$$

This results is inserted in Eq. (72):

$$i\partial_t \left(\hat{\Omega}_{in}(t)\hat{\Omega}_{out}^{-1}(t) \right) = \hat{V}_{in}(t)\hat{\Omega}_{in}(t)\hat{\Omega}_{out}^{-1}(t) - \hat{\Omega}_{in}(t)\hat{\Omega}_{out}^{-1}(t)\hat{V}_{out}(t) \tag{75}$$

A picture transformation like stated for the Interaction picture in Eq. (17) allows us to write both potentials in the Heisenberg representation.

$$i\partial_t\hat{S} = \hat{\Omega}_{in}(t)\hat{V}_H\hat{\Omega}_{out}^{-1}(t) + \hat{\Omega}_{in}(t)(-\hat{V}_H)\hat{\Omega}_{out}^{-1}(t) = 0. \tag{76}$$

This time independence of the product gives us the choice to set t to any value. In particular by setting it to $t = \infty$ we find that Eq. (71) reduces to

$$\hat{S} = \hat{\Omega}_{in}(\infty), \tag{77}$$

where the initial conditions, $\hat{\Omega}_{out}(\infty) = 1$ has been used. Similarly, if $t = \infty$ we use $\hat{\Omega}_{in}(-\infty) = 1$ and

$$\hat{S} = \hat{\Omega}_{out}^{-1}(-\infty), \tag{78}$$

Taking into account, that a lot of literature around quantum field theory relates the $\hat{S}$ operator in term of the Interaction picture, we shall verify a

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secondary set of relations. Starting in a state in the *in* picture, we go to the Heisenberg and then to the Interaction picture similar to what we have done in Eq. (71).

$$
\begin{aligned}
|\Psi_{in}(t)\rangle &= \hat{\Omega}_{in}(t) |\Psi_H\rangle \\
&= \hat{\Omega}_{in}(t)\hat{\Omega}_I^{-1}(t) |\Psi_I(t)\rangle .
\end{aligned}
\tag{79}
$$

This new product of unitary operators is also time independent. This can be shown by taking the partial derivative as seen in Eq. (72). The derivative of the inverse operator $\left[\dot{\hat{\Omega}}_I^{-1}(t)\right]$ will also result in a $-\hat{V}_H\hat{\Omega}_I^{-1}(t)$. Thus,

$$
i\partial_t\hat{\Omega}_{in}(t)\hat{\Omega}_I^{-1}(t) = \hat{\Omega}_{in}(t)\hat{V}_H\hat{\Omega}_I^{-1}(t) + \hat{\Omega}_{in}(t)(-\hat{V}_H)\hat{\Omega}_I^{-1}(t) = 0.
\tag{80}
$$

To bring the $\hat{S}$ operator into our equation, we substitute $\hat{\Omega}_{in}(t)$ using the definition in Eq. (71):

$$
\hat{\Omega}_{in}(t)\hat{\Omega}_I^{-1}(t) = \hat{S}\hat{\Omega}_{out}(t)\hat{\Omega}_I^{-1}(t).
\tag{81}
$$

We can set t to the initial condition of a picture now including $\hat{\Omega}_I(0) = 1$, since we have verified time independence.

$$
\begin{aligned}
\hat{\Omega}_{in}(t)\hat{\Omega}_I^{-1}(t) &= \hat{S} \ \hat{\Omega}_I^{-1}(\infty) \\
&= \hat{\Omega}_{in}(0).
\end{aligned}
\tag{82}
$$

Finally, we want to derive the following expression:

$$
\hat{\Omega}_{in}(t) = \bar{T}\left(e^{i\int_t^\infty \mathrm{d}t'\hat{V}_{in}(t')}\right)\hat{S}.
\tag{83}
$$

This formula is essential in our way of establishing the Gell-Mann Low formula, which is carried out in the next section. First it must satisfy the differential equation for $\hat{\Omega}_{in}(t)$ [see Eq. (45)]. To reduce the number of integrals directly depending on t to one, we use the representation for the exponential function without anti-chronological time ordering similar to Eq. (60):

$$
i\partial_t\hat{\Omega}_{in}(t) = i\partial_t\left(\sum_n i^n \int_t^\infty \mathrm{d}t_1\hat{V}_{in}(t_1)\dots\int_{t_{n-1}}^\infty \mathrm{d}t_n\hat{V}_{in}(t_n)\right)\hat{S}.
\tag{84a}
$$

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The Leibniz integral rule can be applied to obtain,

$$i\partial_t \hat{\Omega}_{in}(t) = i \left(\sum_n i^n \left(-\hat{V}_{in}(t)\right) \int_{t_1}^{\infty} dt_2 \hat{V}_{in}(t_2) \ldots \int_{t_{n-1}}^{\infty} dt_n \hat{V}_{in}(t_n) \right) \hat{S}.$$

(84b)

An i taken out of the sum allows us to remove the negative sign and restores the correct power $n-1$. By using the definition of anti-chronological time ordering (see appendix 5.A) and changing the summation index ($n - 1 = \tilde{n}$),

$$i\partial_t \hat{\Omega}_{in}(t) = \hat{V}_{in}(t) \sum_{\tilde{n}=1}^{\infty} \frac{i^{\tilde{n}}}{\tilde{n}!} \int_{t'_0}^{\infty} dt'_1 \ldots \int_{t'_0}^{\infty} dt'_{\tilde{n}} \bar{T}\left(\hat{V}_{in}(t'_1) \ldots \hat{V}_{in}(t'_{\tilde{n}})\right) \hat{S}. \quad (85)$$

$$i\partial_t \hat{\Omega}_{in}(t) = \hat{V}_{in}(t) \underbrace{\bar{T}\left(e^{i \int_t^{\infty} dt' \hat{V}_{in}(t')}\right) \hat{S}}_{=\hat{\Omega}_{in}(t)}.$$

(86)

Now we verify that the initial condition $\left[\hat{\Omega}_{in}(-\infty) = 1\right]$ still holds for the representation given in Eq. (83). For this we evaluate it as follows:

$$\hat{\Omega}_{in}(-\infty) = \bar{T}\left(e^{i \int_{-\infty}^{\infty} dt' \hat{V}_{in}(t')}\right) \hat{S} \qquad (87)$$

At this point we need to make use of an important property of the time ordered operators.

The hermitian conjugation of anti-chronological time ordering of a product of operators $\hat{V}(t)$ turns it into the chronological time ordering of same operators, as long as $\hat{V}(t)$ is hermitian. Note that this can be seen immediately by taking the hermitian conjugate of Eq. (61):

$$\left[\bar{T}(\hat{V}(t_1) \ldots \hat{V}(t_n))\right]^{\dagger} = T(\hat{V}(t_1) \ldots \hat{V}(t_n)). \qquad (88)$$

By keeping this in mind, we can recognize in Eq. (87) the hermitian conjugate of Eq. (65) evaluated at $t = \infty$:

$$\hat{\Omega}_{in}(-\infty) = (\hat{\Omega}_{in}(\infty))^{\dagger} \hat{S}$$
$$\underbrace{=}_{\text{Eq. (77)}} \hat{S}^{-1}\hat{S} = 1, \qquad (89)$$

where the last step relies on the unitary of $\hat{S}$. This can be seen straight away by taking the hermitian conjugate of Eq. (71).

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3.3   Gell-Mann Low formula

Recalling Eq. (17) we can write:

$$\hat{Q}_H(t) = \hat{\Omega}_I(t)^{-1}\hat{Q}_I(t)\,\hat{\Omega}_I(t). \tag{90}$$

Let us consider Eq. (17) with the initial condition taken at $t \to -\infty$:

$$\hat{Q}_H(t) = \hat{\Omega}_{in}(t)^{-1}\hat{Q}_{in}(t)\,\hat{\Omega}_{in}(t). \tag{91}$$

Expressing $\hat{\Omega}_{in}^{-1}(t)$ using Eq. (83) and $\hat{\Omega}_{in}(t)$ as in Eq. (65). We find

$$\hat{Q}_H(t) = \left[\bar{T}\left(e^{i\int_t^\infty dt'\hat{V}_{in}(t')}\right)\hat{S}\right]^{-1}\hat{Q}_{in}(t)T\left(e^{-i\int_{-\infty}^t dt'\hat{V}_{in}(t')}\right). \tag{92}$$

Since $\hat{\Omega}_{in}(t)$ is a unitary operator we can replace its inverse by its hermitian conjugate:

$$\hat{Q}_H(t) = \hat{S}^{-1}\left[\bar{T}\left[e^{i\int_t^\infty dt'\hat{V}_{in}(t')}\right]\right]^\dagger\hat{Q}_{in}(t)T\left(e^{-i\int_{-\infty}^t dt'\hat{V}_{in}(t')}\right), \tag{93a}$$

where the unitarity of $\hat{S}$ has been used. Taking Eq. (88) into account, this expression can be written as

$$\hat{Q}_H(t) = \hat{S}^{-1}T\left(e^{-i\int_t^\infty dt'\hat{V}_{in}(t')}\right)\hat{Q}_{in}(t)T\left(e^{-i\int_{-\infty}^t dt'\hat{V}_{in}(t')}\right). \tag{94}$$

The trivial case $\hat{Q}_H(t) = T\left[\hat{Q}_H(t)\right]$ allows us to apply the chronological time ordering to the entire right-hand side.

$$\hat{Q}_H(t) = T\left[\hat{S}^{-1}T\left(e^{-i\int_t^\infty dt'\hat{V}_{in}(t')}\right)\hat{Q}_{in}(t)T\left(e^{-i\int_{-\infty}^t dt'\hat{V}_{in}(t')}\right)\right]. \tag{95}$$

In the next step we can move $\hat{S}^{-1}$ out of the exterior time ordering. This is allowed since it fulfils the conditions of time independence and the key point at this moment: it has <u>not</u> been involved or is a result of commutations, that are only equal to 1 due to the now present exterior time ordering. Therefore we write:

$$\hat{Q}_H(t) = \hat{S}^{-1}T\left[T\left(e^{-i\int_t^\infty dt'\hat{V}_{in}(t')}\right)\hat{Q}_{in}(t)T\left(e^{-i\int_{-\infty}^t dt'\hat{V}_{in}(t')}\right)\right]. \tag{96}$$

As explained in the appendix 5.A inside of time ordering operator commutators can be kept to 0. We will use it to move $\hat{Q}_{in}(t)$ to

$$\hat{Q}_H(t) = \hat{S}^{-1}T\left[\hat{Q}_{in}(t)T\left(e^{-i\int_t^\infty dt'\hat{V}_{in}(t')}\right)T\left(e^{-i\int_{-\infty}^t dt'\hat{V}_{in}(t')}\right)\right]. \tag{97}$$

To fuse the two inner T operators, we need to establish under which conditions operators can be moved inside of an already time ordered expression. Let's consider a case with an arbitrary operator $\hat{M}(t)$:

$$\hat{M}(t)T\left(e^{-i\int_{-\infty}^{t}\mathrm{d}t'\hat{V}_{in}(t')}\right). \tag{98}$$

We use the non compact and non symbolic expression for $\hat{\Omega}_{in}(t)$ similar to Eq. (56). Focused on the term for $n = 2$, we write

$$\frac{1}{2}\hat{M}(t)\int_{-\infty}^{t}\mathrm{d}t'_1\int_{-\infty}^{t}\mathrm{d}t'_2 T\left(\hat{V}_{in}(t'_1)\hat{V}_{in}(t'_2)\right)$$
$$= \int_{-\infty}^{t}\mathrm{d}t'_1\int_{-\infty}^{t'_1}\mathrm{d}t'_2\hat{M}(t)\hat{V}_{in}(t'_1)\hat{V}_{in}(t'_2). \tag{99}$$

We see that this product has the operator $\hat{M}(t)$ already at the chronological time ordered position, because the variable t is fixed as the latest time by the integral limits.

This can be formulated into a condition. Any operator $\hat{M}(t)$ multiplied from the left (right) can be moved into a chronological time ordered product dependent on a number of t_i variables , if it can be guaranteed that $t < t_i$ ($t > t_i$). Thus the correct time ordered position of $\hat{M}(t)$ is at the head or tail of the set. Keeping this in mind it is sufficient for an overall chronological time ordering to multiply with the Heaviside function depended only on t'_1 and t'_1.

$$\frac{1}{2}\int_{-\infty}^{t}\mathrm{d}t'_1\int_{-\infty}^{t}\mathrm{d}t'_2\hat{M}(t)\hat{V}_{in}(t'_1)\hat{V}_{in}(t'_2)\theta(t'_1 - t'_2)$$
$$+ \frac{1}{2}\int_{-\infty}^{t}\mathrm{d}t'_1\int_{-\infty}^{t}\mathrm{d}t'_2\hat{M}(t)\hat{V}_{in}(t'_1)\hat{V}_{in}(t'_2)\theta(t'_2 - t'_1) \tag{100}$$
$$= \frac{1}{2}\int_{-\infty}^{t}\mathrm{d}t'_1\int_{-\infty}^{t}\mathrm{d}t'_2 T\left[\hat{M}(t)\hat{V}_{in}(t'_1)\hat{V}_{in}(t'_2)\right].$$

The condition for extending the operator T in products is fulfilled for each term in the expression $\hat{\Omega}_{in}(t)$, where the limit 0 is taken to $-\infty$ in Eq. (56). Therefore we can write:

$$\hat{M}(t)T\left(e^{-i\int_{-\infty}^{t}\mathrm{d}t'\hat{V}_{in}(t')}\right) = T\left(\hat{M}(t)e^{-i\int_{-\infty}^{t}\mathrm{d}t'\hat{V}_{in}(t')}\right). \tag{101}$$

Coming back to our expression for $\hat{Q}_H(t)$, we want to extend the right inner T over both exponential functions. To apply Eq. (101) we expand the left exponential function. To keep the expression to a comprehensible length, we just focus on the exterior time ordering and both exponential functions taken from Eq. (97)

$$T\left[T\left(e^{-i\int_t^\infty dt'\hat{V}_{in}(t')}\right)T\left(e^{-i\int_{-\infty}^t dt'\hat{V}_{in}(t')}\right)\right]$$
$$= T\left[\left(\sum_n(-i)^n\int_t^\infty dt'_1\ldots\int_{t'_{n-1}}^\infty dt'_n\hat{V}_{in}(t'_1)\ldots\hat{V}_{in}(t'_n)\right)T\left(e^{-i\int_{-\infty}^t dt'\hat{V}_{in}(t')}\right)\right].$$
$$(102)$$

We see that each term in the series fulfils the condition to be moved into the inner time ordering. In addition the external time ordering would made it possible to commute all $\hat{V}_{in}(t'_i)$ if necessary. Inside the inner T operator we write the compact notation

$$T\left[T\left(e^{-i\int_t^\infty dt'\hat{V}_{in}(t')}e^{-i\int_{-\infty}^t dt'\hat{V}_{in}(t')}\right)\right]$$
$$= T\left[T\left(e^{-i\int_t^\infty dt'\hat{V}_{in}(t')-i\int_{-\infty}^t dt'\hat{V}_{in}(t')}\right)\right].$$
$$(103)$$

In the last step the BCH-formula has been used and due to the chronological time ordering, we could set the appearing commutator to zero.

By taken all step together we can write Eq. (94) in the form:

$$\hat{Q}_H(t) = \hat{S}^{-1}T\left[\hat{Q}_{in}(t)T\left(e^{-i\int_t^\infty dt'\hat{V}_{in}(t')-i\int_{-\infty}^t dt'\hat{V}_{in}(t')}\right)\right]. \qquad (104)$$

We can apply the expression for $\hat{S}$ given in the second line of Eq. (77) as long as we keep the scattering operator inside the time ordering, since several non trivial commutations have been performed in the derivation. These are only ensured to be equal to 1 inside of the chronological time ordering.

$$\hat{Q}_H(t) = \hat{S}^{-1}T\left[\hat{Q}_{in}(t)\hat{S}\right]. \qquad (105)$$

Next will be case for more than one operator. We start with the left side in chronological time ordering and apply Eq. (105) to each $\hat{Q}_H(t_j)$. This results in

$$T\left[\prod_j^n\hat{Q}_H(t_j)\right] = T\left[\prod_j^n\hat{S}^{-1}T\left(\hat{Q}_{in}(t_j)\hat{S}\right)\right]. \qquad (106)$$

Over the entire product all we can cancel $\hat{S}$ and $\hat{S}^{-1}$ by moving the inverted scattering operator into the inner time ordering on their left side. This is allowed due to them being time independent and the exterior T operator. Reducing the expression to

$$
\begin{aligned}
T\left[\prod_j^n \hat{Q}_H(t_j)\right] &= T\left[\hat{S}^{-1}\prod_j^n T\left(\hat{Q}_{in}(t_j)\hat{S}\right)\right] \\
&= \hat{S}^{-1}T\left[\prod_j^n T\left(\hat{Q}_{in}(t_j)\hat{S}\right)\right].
\end{aligned}
\tag{107}
$$

In the second line we moved the $\hat{S}^{-1}$ operator out of the exterior time ordering same as in Eq. (95) . The inner T operator can be dropped as due to the overall chronological time ordering. From this we arrive at the final form of the Gell-Mann Low formula:

$$
T\left(\hat{Q}_H(t_1)\hat{Q}_H(t_2)\ldots\right) = \hat{S}^{-1}T\left(\hat{Q}_{in}(t_1)\hat{Q}_{in}(t_2)\ldots\hat{S}\right).
\tag{108}
$$

Its major importance in quantum field theory comes from the central role in many perturbation calculations. When applied between asymptotic vacuum states of the *in* and *out* picture, it reads:

$$
\begin{aligned}
&\langle 0_{out}|\, T\left(\hat{Q}_H(t_1)\hat{Q}_H(t_2)\ldots\right)|0_{in}\rangle \\
&= \langle 0_{out}|\,\hat{S}^{-1}T\left(\hat{Q}_{in}(t_1)\hat{Q}_{in}(t_2)\ldots\hat{S}\right)|0_{in}\rangle
\end{aligned}
\tag{109}
$$

The scattering operator allows to transform these asymptotic states like:

$$
\langle 0_{out}|\,\hat{S}^{-1} = \frac{\langle 0_{in}|}{\langle 0_{out}|0_{in}\rangle},
\tag{110}
$$

where the nominator is equal to 1 for stable vacua. Substituting Eq. (110) in (109) gives

$$
\begin{aligned}
&\langle 0_{out}|\, T\left(\hat{Q}_H(t_1)\hat{Q}_H(t_2)\ldots\right)|0_{in}\rangle \\
&= \frac{\langle 0_{in}|\, T\left(\hat{Q}_{in}(t_1)\hat{Q}_{in}(t_2)\ldots\hat{S}\right)|0_{in}\rangle}{\langle 0_{out}|0_{in}\rangle} \\
&= \frac{\langle 0_{in}|\, T\left(\hat{Q}_{in}(t_1)\hat{Q}_{in}(t_2)\ldots e^{-i\int_{-\infty}^{\infty}\mathrm{d}t\,\hat{V}_{in}(t')}\right)|0_{in}\rangle}{\langle 0_{out}|0_{in}\rangle}
\end{aligned}
\tag{111}
$$

This exponential function can now be treated in a pertubation using the Wick Theorem.

4 Wick theorem and vacuum stability

The Wick theorem as a means to evaluate correlation functions, can be established by further investigating the $\hat{S}$ operator. In section 2.3, the Eq. (43) expressed the potential term of our full Hamiltonian in the Interaction picture. Going to the *in* picture, we write $\hat{V}_{in} = \sum_k \bar{j}_{\underline{k}}(t)\hat{q}_{\underline{k},in}(t)$. Using $\hat{S} = \hat{\Omega}_{in}(\infty)$ (see Eq. (77)) and taking (65) into account, an expression in term of the current can be formulated.Explicitly,

$$\hat{S} = T\left[\exp\left(i\sum_{\underline{k}}\int dt\ \bar{j}_{\underline{k}}(t)\hat{q}_{\underline{k},in}(t)\right)\right] \tag{112a}$$

$$\stackrel{\text{Eq.(32)}}{=} T\left[\exp\left(i\sum_{\underline{k}}\int dt\ \bar{j}_{\underline{k}}(t)\frac{1}{2\omega_{\underline{k}}}\left(\hat{a}_{\underline{k},in}e^{-i\omega_{\underline{k}}t} + \hat{a}^{\dagger}_{\underline{k},in}e^{i\omega_{\underline{k}}t}\right)\right)\right]. \tag{112b}$$

Using the the BCH-formula, we split the exponent. To simplify we use the temporal Fourier transformation given below Eq. (35). As a consequence,

$$\hat{S} = \exp\left(i\sum_{\underline{k}}\bar{j}_{\underline{k}}(\omega_{\underline{k}})\frac{1}{2\omega_{\underline{k}}}\hat{a}^{\dagger}_{\underline{k},in}\right)\exp\left(i\sum_{\underline{k}}\bar{j}_{\underline{k}}(-\omega_{\underline{k}})\frac{1}{2\omega_{\underline{k}}}\hat{a}_{\underline{k},in}\right)$$
$$\times \exp\left(-\frac{1}{2}\left[i\sum_{\underline{k}}\bar{j}_{\underline{k}}(\omega_{\underline{k}})\frac{1}{2\omega_{\underline{k}}}\hat{a}^{\dagger}_{\underline{k},in}, i\sum_{\underline{k}'}\bar{j}_{\underline{k}'}(-\omega_{\underline{k}'})\frac{1}{2\omega_{\underline{k}'}}\hat{a}_{\underline{k}',in}\right]\right). \tag{113}$$

We note that, in this expression there is no further dependence on t and therefore the T operator has been dropped. We move all common factors

out of the commutator,

$$
\hat{S} = \exp\left(i \sum_{\underline{k}} \bar{j}_{\underline{k}}(\omega_{\underline{k}}) \frac{1}{2\omega_{\underline{k}}} \hat{a}^{\dagger}_{\underline{k},in} \right) \exp\left(i \sum_{\underline{k}} \bar{j}_{\underline{k}}(-\omega_{\underline{k}}) \frac{1}{2\omega_{\underline{k}}} \hat{a}_{\underline{k},in} \right)
$$
$$
\times \exp\left(\sum_{\underline{k},\underline{k}'} \frac{1}{4\omega_{\underline{k}}\omega_{\underline{k}'}} \bar{j}_{\underline{k}}(\omega_{\underline{k}}) \bar{j}_{\underline{k}'}(-\omega_{\underline{k}'}) \left[\hat{a}^{\dagger}_{\underline{k},in}, \hat{a}_{\underline{k}',in} \right] \right). \tag{114}
$$

By using the commutation relation given in Eq. (33):

$$
\hat{S} = \exp\left(i \sum_{\underline{k}} \frac{1}{2\omega_{\underline{k}}} \bar{j}_{\underline{k}}(\omega_{\underline{k}}) \hat{a}^{\dagger}_{\underline{k},in} \right) \exp\left(i \sum_{\underline{k}} \frac{1}{2\omega_{\underline{k}}} \bar{j}_{\underline{k}}(-\omega_{\underline{k}}) \hat{a}_{\underline{k},in} \right)
$$
$$
\times \exp\left(-\sum_{\underline{k}} \frac{1}{4\omega_{\underline{k}}} |\bar{j}_{\underline{k}}(\omega_{\underline{k}})|^2 \right). \tag{115}
$$

In this expression the creation operators $\hat{a}^{\dagger}_{\underline{k},in}$ are placed to the left of the annihilation operators $\hat{a}_{\underline{k},in}$. This is known as "normal" ordering. To keep it this way and making other expressions easier, we introduce a notational symbol to force them to stay so.

It is called the "normal ordering" and we write in a general form:

$$
: aa^{\dagger} : \quad = \quad : a^{\dagger}a : \quad = a^{\dagger}a. \tag{116}
$$

Take notice of the effect on the commutator:

$$
: \left[\hat{a}_{\underline{k},in}, \hat{a}^{\dagger}_{\underline{k},in} \right] : \quad = \quad : \hat{a}_{\underline{k},in}\hat{a}^{\dagger}_{\underline{k},in} : - : \hat{a}^{\dagger}_{\underline{k},in}\hat{a}_{\underline{k},in} :
$$
$$
= \quad : \hat{a}^{\dagger}_{\underline{k},in}\hat{a}_{\underline{k},in} : - : \hat{a}^{\dagger}_{\underline{k},in}\hat{a}_{\underline{k},in} : \tag{117}
$$
$$
= 0
$$

Following this in our case the BCH-formula becomes trivial inside of normal ordering and we can write the product

$$
\exp\left(i \sum_{\underline{k}} \frac{1}{2\omega_{\underline{k}}} \bar{j}_{\underline{k}}(\omega_{\underline{k}}) \hat{a}^{\dagger}_{\underline{k},in} \right) \exp\left(i \sum_{\underline{k}} \frac{1}{2\omega_{\underline{k}}} \bar{j}_{\underline{k}}(-\omega_{\underline{k}}) \hat{a}_{\underline{k},in} \right)
$$
$$
= \quad : \exp\left(i \sum_{\underline{k}} \frac{1}{2\omega_{\underline{k}}} \bar{j}_{\underline{k}}(\omega_{\underline{k}}) \hat{a}^{\dagger}_{\underline{k},in} + i \sum_{\underline{k}} \frac{1}{2\omega_{\underline{k}}} \bar{j}_{\underline{k}}(-\omega_{\underline{k}}) \hat{a}_{\underline{k},in} \right) : . \tag{118}
$$

Or simply,

$$= \quad : \exp\left(i \sum_{\underline{k}} \int dt\ \bar{j}_{\underline{k}}(t)\hat{q}_{\underline{k},in}(t) \right) : . \tag{119}$$

The third exponential function in Eq. (114) can be formulated differently by reversing the temporal Fourier transformation. The exponential functions of the transformation $e^{-iw_{\underline{k}}t}$ will be joined and we take the absolute value of the different times t, t':

$$\exp\left(-\sum_{\underline{k}} \frac{1}{4\omega_{\underline{k}}} |\bar{j}_{\underline{k}}(\omega_{\underline{k}})|^2 \right)$$

$$= \exp\left(-\sum_{\underline{k}} \frac{1}{4\omega_{\underline{k}}} \int dt \int dt'\ \bar{j}_{\underline{k}}(t) e^{-iw_{\underline{k}}|t-t'|} \bar{j}_{\underline{k}}(t') \right). \tag{120}$$

We now introduce the Feynman Green's function for one mode:

$$G_{\underline{k}}(t - t') = \frac{1}{2\omega_{\underline{k}}} e^{-i\omega_{\underline{k}}|t-t'|}. \tag{121}$$

By substituting Eq. (121) into Eq. (120), we find the second exponential function required for re-expressing the $\hat{S}$-operator. With this one and Eq. (119) we can establish the relation in term of the modes of a real scalar field.

$$\hat{S} = T\left[\exp\left(i\sum_{\underline{k}} \int dt\ \bar{j}_{\underline{k}}(t)\hat{q}_{\underline{k},in}(t) \right) \right] = \quad : \exp\left(i\sum_{\underline{k}} \int dt\ \bar{j}_{\underline{k}}(t)\hat{q}_{\underline{k},in}(t) \right) :$$

$$\times \exp\left(-\frac{1}{2}\sum_{\underline{k}} \int dt \int dt'\ \bar{j}_{\underline{k}}(t) G_{k}(t - t') \bar{j}_{\underline{k}}(t') \right). \tag{122}$$

One can easily derive this expression in terms of the quantized field $\hat{\Phi}$. It follows from the inversion of Eq. (24), $\hat{q}_{\underline{k}}(t) = \int dx\ \hat{\Phi}(\underline{x}, t) u^{\star}_{\underline{k}}(\underline{x})$ and its substitution in Eq. (122). A repeated use of the completeness relation in

Eq. (27) lead us to:

$$\hat{S} = T\left[\exp\left(i\int d^4x\, j(x)\Phi(x)\right)\right] = \ :\exp\left(i\int d^4x\, j(x)\Phi(x)\right): $$
$$\times \exp\left(-\frac{1}{2}\int d^4x\int d^4x'\, j(x)\triangle_F(x-x')j(x')\right), \tag{123}$$

where $\triangle_F(x-x')$ is the Feynman propagator for the real scalar field. It reads in the covariant form:

$$\triangle_F(x - x') = \int \frac{d^4k}{(2\pi)^4}\frac{i}{k^2 - m^2 + i\epsilon}e^{-ik(x-x')}. \tag{124}$$

Here ϵ is a positive infinitesimal and $k^2 = \omega_{\underline{k}}^2 - \underline{k}^2$. Eq. (123) in combination with functional derivatives respect the currents of the regarded theory and taking the vacuum expectation value, allows us to find the desired correlations functions. For example the time ordered product of two fields $\hat{\Phi}(x_1)$ and $\hat{\Phi}(x_2)$ can be obtained from the generating functional given in Eq. (123) by taken the functional derivatives $\delta/\delta j(x_1)$ and $\delta/\delta j(x_2)$, while afterwards setting the current to zero:

$$T\left(\hat{\Phi}(x_1)\hat{\Phi}(x_2)\right) = \ :\hat{\Phi}(x_1)\hat{\Phi}(x_2): +\triangle_F(x_1 - x_2). \tag{125}$$

This relation is called the *Wick theorem* and can be extended to any finite number of field operators.

Beside obtaining the Wick theorem, we can use Eq. (115) to verify that, in the presence of an external current, the vacuum is not stable. For showing this we compute the probability for staying in the ground state:

$$p_0 = |\langle 0_{out}|0_{in}\rangle|^2 = \left|\langle 0_{in}|\hat{S}|0_{in}\rangle\right|^2 \tag{126a}$$

$$= \left|\langle 0_{in}|e^{\sum_{\underline{k}}\frac{i}{2\omega_{\underline{k}}}\bar{j}_{\underline{k}}(\omega_{\underline{k}})\hat{a}_{\underline{k},in}^\dagger}\, e^{\sum_{\underline{k}}\frac{i}{2\omega_{\underline{k}}}\bar{j}_{\underline{k}}(-\omega_{\underline{k}})\hat{a}_{k,in}}\, e^{\sum_{\underline{k}}-\frac{1}{4\omega_{\underline{k}}}|\bar{j}_{\underline{k}}(-\omega_{\underline{k}})|^2}|0_{in}\rangle\right|^2. \tag{126b}$$

The annihilation operator will return a 0 in the exponent. Therefore only one factor remain important. It reads:

$$p_0 = \exp\left\{-\int\frac{d^3k}{(2\pi)^3}\left|\frac{\bar{j}_{\underline{k}}(\omega_{\underline{k}})}{\sqrt{2\omega_{\underline{k}}}}\right|^2\right\}. \tag{127}$$

Here we have made a transition the continuous description of the modes of our field by replacing the sum with an integral. This confirms our statement about an unstable vacuum. The negative sign in the exponent translates to smaller probabilities $(p_0 < 1)$.

5 Conclusion

In this report we have presented a set of fundamental concepts and methods. These are essential for starting to study Quantum field theory. We began with well-known pictures from quantum mechanics and introduced the *in* and *out* picture as consequences of working with asymptotic states found by investigating the effect of an external current on an scalar action. Establishing connections between the pictures on the level of interaction states was based on the scattering operator $\hat{S}$. From it the Wick theorem as well as the vacuum instability could be verified. At last it allowed us to derive the Gell-Mann Low formula, which plays a major part in the second quantisation performed in context of quantum field theory.

5.A Chronological and Anti-Chronological time ordering

To expand our concept of chronological time ordering to cases of more then two t we start by advancing the definition stated in Eq. (54). In general it consists of a summation of all permutations P of a given set multiplied by Heaviside functions. These Heaviside functions have arguments with the negative summation of the t in the same permutation P. We keep the number of brackets low by denoting $\hat{V}_I(t_1) \to \hat{V}_1$

Definition:

$$T(\hat{V}_1, \hat{V}_2, \ldots, \hat{V}_n) = \sum_{j=1}^{n!} P_j \left[\hat{V}_1, \hat{V}_2, \ldots, \hat{V}_n \right] \cdot \theta \left(P_j \left[t_j - \sum_{i \neq j}^{n} t_i \right] \right) \quad . \quad (128)$$

The generalisation of anti-chronological time ordering given in Eq. (61) is based on the same principle. The main difference lays in the t_i in the argument of Heaviside function, which is not multiplied by -1. Definition:

$$\bar{T}(\hat{V}_1, \hat{V}_2, \ldots, \hat{V}_n) = \sum_{j=1}^{n!} P_j \left[\hat{V}_1, \hat{V}_2, \ldots, \hat{V}_n \right] \cdot \theta \left(P_j \left[t_{n-j+1} - \sum_{i \neq j}^{n} t_i \right] \right) \quad . \tag{129}$$

As a test we set $n = 3$ in Eq. (128):

$$\begin{aligned}
T(\hat{V}_1, \hat{V}_2, \hat{V}_3) &= \sum_{j=1}^{3!} P_j \left[\hat{V}_1, \hat{V}_2, \hat{V}_3 \right] \cdot \theta \left(P_j \left[t_j - \sum_{i \neq j}^{3} t_i \right] \right) \\
&= \hat{V}_1 \hat{V}_2 \hat{V}_3 \cdot \theta(t_1 - t_2 - t_3) \\
&\quad + \hat{V}_1 \hat{V}_3 \hat{V}_2 \cdot \theta(t_1 - t_3 - t_2) \\
&\quad + \hat{V}_2 \hat{V}_1 \hat{V}_3 \cdot \theta(t_2 - t_1 - t_3) \\
&\quad + \hat{V}_2 \hat{V}_3 \hat{V}_1 \cdot \theta(t_2 - t_3 - t_1) \\
&\quad + \hat{V}_3 \hat{V}_1 \hat{V}_2 \cdot \theta(t_3 - t_1 - t_2) \\
&\quad + \hat{V}_3 \hat{V}_2 \hat{V}_1 \cdot \theta(t_3 - t_2 - t_1).
\end{aligned} \tag{130}$$

As well as $n = 3$ in Eq. (129)

$$\bar{T}(\hat{V}_1, \hat{V}_2, \hat{V}_3) = \sum_{j=1}^{3!} P_j \left[\hat{V}_1, \hat{V}_2, \hat{V}_3 \right] \cdot \theta \left(P_j \left[t_{n-j+1} - \sum_{i \neq j}^{3} t_i \right] \right)$$
$$= \hat{V}_1 \hat{V}_2 \hat{V}_3 \cdot \theta(t_3 - t_2 - t_1)$$
$$+ \hat{V}_1 \hat{V}_3 \hat{V}_2 \cdot \theta(t_2 - t_3 - t_1)$$
$$+ \hat{V}_2 \hat{V}_1 \hat{V}_3 \cdot \theta(t_3 - t_1 - t_2) \tag{131}$$
$$+ \hat{V}_2 \hat{V}_3 \hat{V}_1 \cdot \theta(t_1 - t_3 - t_2)$$
$$+ \hat{V}_3 \hat{V}_1 \hat{V}_2 \cdot \theta(t_2 - t_1 - t_3)$$
$$+ \hat{V}_3 \hat{V}_2 \hat{V}_1 \cdot \theta(t_1 - t_2 - t_3).$$

The following results and calculations can be performed in the same fashion for chronological and anti-chronological time ordering. We will show them explicitly for the case of chronological time ordering.

In Eq. (51) we defined an function $I(t)$ for two potentials $V_I(t)$. Expanding this function to the case of n requires a a normalization factor alongside T. From stochastic we know a set of n different elements can be linear arranged in $n!$ ways. Therefore a factor of $1/n!$ in the expressions for $I(t)$ is required, when ever chronological time ordering is applied.

Now we use Eq. (128) in a larger $I(t)$ and perform a proof by induction based on the number of $\hat{V}$. The induction start is the case of two $\hat{V}$. In the induction step we state that it works for at least one unspecified higher order. Let's call it k : (*Note: $t_0 = t$*)

$$I_k(t) = \prod_{a=1}^{k} \int_{-\infty}^{t_{a-1}} dt_a \; \hat{V}_a = \frac{1}{k!} (\prod_{a=1}^{k} \int_{-\infty}^{t} dt_a \;) T(\hat{V}_1, \ldots, \hat{V}_k). \tag{132}$$

Moving one increment higher in our 'chain' $k + 1$:

$$I_{k+1}(t) = \prod_{a=1}^{k+1} \int_{-\infty}^{t_{a-1}} dt_a \; \hat{V}_a = \prod_{a=1}^{k} \int_{-\infty}^{t_{a-1}} dt_a \; \hat{V}_a \cdot \int_{-\infty}^{t_k} dt_{k+1} \; \hat{V}_{k+1}. \tag{133}$$

Using the Induction Step and general definition Eq. (128):

$$I_{k+1}(t) = \frac{1}{k!} (\prod_{a=1}^{k} \int_{-\infty}^{t} dt_a \;) T(\hat{V}_1, \ldots, \hat{V}_k) \cdot \int_{-\infty}^{t_k} dt_{k+1} \; \hat{V}_{k+1} \tag{134}$$

$$I_{k+1}(t) = I_k(t) \cdot \int_{-\infty}^{t_k} \mathrm{d}t_{k+1} \ \hat{V}_{k+1} \tag{135}$$

This shows that the incrementation of k reduces to a multiplication with one more different element to the set. This increases the possible permutations by a factor of $k+1$ resulting in $(k+1)!$ in total. Giving us:

$$I_{k+1}(t) = \frac{1}{(k+1)!} \left(\prod_{a=1}^{k+1} \int_{-\infty}^{t} \mathrm{d}t_a \right) T(\hat{V}_1, \dots, \hat{V}_{k+1}) \tag{136}$$

An very useful aspect of chronological as well as anti-chronological time ordering is all operators V_i in $T(\dots)$ or $\bar{T}(\dots)$ commute. For two elements:

$$T(\hat{V}_1, \hat{V}_2) = \hat{V}_1 \ \hat{V}_2 \ \theta(t_1 - t_2) \ + \ \hat{V}_2 \ \hat{V}_1 \ \theta(t_2 - t_1) \tag{137a}$$

$$T(\hat{V}_2, \hat{V}_1) = \hat{V}_2 \ \hat{V}_1 \ \theta(t_2 - t_1) \ + \ \hat{V}_1 \ \hat{V}_2 \ \theta(t_1 - t_2), \tag{137b}$$

after switching the terms,

$$T(\hat{V}_1, \hat{V}_2) = T(\hat{V}_2, \hat{V}_1) \tag{138}$$

In other words, the commutation relations say whether the subtraction of permutations of elements is zero or not. But in time ordering all permutations appear, we can rearrange the terms so subtraction of equal permutations happens. Therefore commutation holds for more then two V_i.

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