Lecture 8

The Klein-Gordon equation

WS2010/11: 'Introduction to Nuclear and Particle Physics'
Bosons with spin 0 $\leftrightarrow$ scalar (or pseudo-scalar) meson fields

canonical field quantization $\Rightarrow$ transition to quantum field theory

- Fock representation for the quantum system of many particles (bosons)
- particle interpretation of the quantum field
  = field quantization (particle counting)
- antiparticles – components of the field itself that can be distinguished in four-momentum representation
The scalar meson field

**Goal:** to determine the fundamental equation of motion for a field $\Phi(R,t)$. $\Phi(R,t)$ is a scalar field for relativistic, spinless particles of nonzero mass $m = \text{meson field}$. 

To determine the fundamental equation of motion, one starts from the requirement that for the Fourier components $\Phi(q,\omega)$ - in the plane-wave representation

$$\Phi(x) = \Phi(r, t) = \frac{1}{(2\pi)^2} \int_{-\infty}^{\infty} d\omega \int d^3q \exp[-i(\omega t - q \cdot r)] \Phi(q, \omega) \quad (1)$$

- the frequency $\omega$ and wave number $q$ are related by the de Broglie relations

$$E = \hbar \omega, \quad p = \hbar q \quad (2)$$

**giving the relativistic energy-momentum relation**

$$E = \pm \sqrt{(cp)^2 + (mc^2)^2} \quad (3)$$

In the system of natural units ($\hbar = c = 1$)

$$\omega = \sqrt{q^2 + m^2} \equiv \omega_q \quad (4)$$

The four-scalar in eq.(1)

$$\omega t - q \cdot r = q_0 x^0 + \sum_{k=1}^{3} q_k x^k = q_\mu x^\mu = q \cdot x \quad (5)$$

is invariant under (proper) Lorentz transformations.
The condition (3) can be written as (mass shell condition)

\[(q^0)^2 - q^2 = q_\mu q^\mu \equiv q^2 = m^2\]  \hspace{1cm} (6)

\[\Phi(q) = \frac{1}{\sqrt{2\pi}} \delta(q_\mu q^\mu - m^2) \chi(q)\]  \hspace{1cm} (7)

and using that

\[\delta(a^2 - b^2) = \frac{1}{2|b|} [\delta(a - b) + \delta(a + b)]\]

\[\Phi(q) = \frac{1}{2\omega_q \sqrt{2\pi}} [\delta(q^0 - \omega_q)\chi_+(q) + \delta(q^0 + \omega_q)\chi_-(q)].\]  \hspace{1cm} (8)

Now integrate (1) over \(d\omega = dq^0\)

\[\Phi(x) = \int \frac{d^3q}{2\omega_q} [\chi_+(q)f_q(x) + \chi_-(q)f_q^*(x)]\]  \hspace{1cm} (9)

with the plane wave basis states

\[f_q(x) = (2\pi)^{-3/2} \exp(-i(\omega_q t - q \cdot r)) = (2\pi)^{-3/2} \exp(-iq \cdot x)|_{q_0 = \omega_q},\]

\[f_q^*(x) = (2\pi)^{-3/2} \exp(i(\omega_q t - q \cdot r)) = (2\pi)^{-3/2} \exp(iq \cdot x)|_{q_0 = \omega_q}.\]  \hspace{1cm} (10)

denoting waves moving forward and backward in space-time.
The Klein-Gordon equation

In the space-time representation (9) the quantity \(-q^2\) is represented by the differential operator (d'Alembert operator)

\[
\frac{\partial}{\partial t^2} - \Delta^2 = \frac{\partial}{\partial x^\mu} \frac{\partial}{\partial x_\mu} = \partial_\mu \partial^\mu
\]  

(11)

From the mass shell condition (6) this results in the **Klein-Gordon equation**

\[
(\partial_\mu \partial^\mu + m^2)\Phi(x) = 0
\]  

(12)

as the basic field equation of the scalar field.

- The plane waves (10) are basic solutions and the field (9) is constructed by a general superposition of the basic states.
- The orthonormalization relation for the plane waves (10) is

\[
(f_q, f_{q'}) = 2\omega_q \delta^3(q - q'),
\]

(13)

where the inner product \((f, g)\) in the relativistic case is defined by

\[
(f, g) = i \int d^3x \left[ f^*(x) \frac{\partial g(x)}{\partial x^0} - \frac{\partial f^*(x)}{\partial x^0} g(x) \right]
\]  

(14)
The scalar product (14) is in general time dependent, since only an integration about $d^3x$ is involved.

Due to (12) a four-current density can be defined as

$$j(x) = \{\rho(r, t), j(r, t)\}$$  \hspace{1cm} (15)

or in covariant notation

$$j^\mu(x) = i \left[ \Phi^*(x) \partial^\mu \Phi(x) - \partial^\mu \Phi^*(x) \Phi(x) \right]$$  \hspace{1cm} (16)

The divergence of the four-current vanishes according to the KG equation

$$\partial_\mu j^\mu(x) \equiv \left( \frac{\partial \rho}{\partial t} + \nabla \cdot j \right) = i \partial_\mu \left[ \Phi^*(x) \partial^\mu \Phi(x) - \partial^\mu \Phi^*(x) \Phi(x) \right]$$  \hspace{1cm} (17)

$$= i \left[ \Phi^*(x) \partial_\mu \partial^\mu \Phi(x) - \partial_\mu \partial^\mu \Phi^*(x) \Phi(x) \right] = -i[m^2 - m^2] \Phi^*(x) \Phi(x) = 0.$$

Note, the density

$$\rho(x) = i \left[ \Phi^*(x) \frac{\partial \Phi(x)}{\partial t} - \frac{\partial \Phi^*(x)}{\partial t} \Phi(x) \right]$$  \hspace{1cm} (18)

is not positive definite and vanishes even for real $\Phi(x)$ fully.

⇒ The field $\Phi(x)$ is therefore not suitable as a probability amplitude!
Quantization

The quantization of the field $\Phi(x)$ assumes that the values of the field at space-time point $x$ are considered as the amplitude of the coordinates $q_i(t)$ in classical mechanics. Analogous to the Hamilton mechanics (and Quantum mechanics) one defines first canonically conjugate momenta by

$$p_i(t) = \frac{\partial L}{\partial \dot{q}_i} \quad i = 1, \ldots, 3N$$  \hspace{1cm} (19)

To do so the knowledge of a Lagrangian $L = L(q_i, \dot{q}_i; t)$  \hspace{1cm} (20)

is required, which by application of Hamilton's principle ($\delta S = 0$, $S$ is the action) gives the equations of motion of the system:

$$\frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}_i} \right) = \frac{\partial L}{\partial q_i}$$  \hspace{1cm} (21)

In quantum mechanics, we then consider the $p_i$ and $q_i$ as operators in Hilbert space - the representation space of the system - and the commutation relation at the same time $t$ in the Heisenberg picture is postulated as:

$$[q_i, p_j] = i\delta_{ij}$$  \hspace{1cm} (22)
The time evolution of the $p_i$ and $q_i$ is given by the equations (21) and all other physical quantities can be calculated from the $q_i$ and $p_i$ after some prescription for the order of the $q_i$ and $p_i$ in the operators. In particular, the Hamiltonian is given by the Legendre transform

$$H = \sum_{i=1}^{3N} \dot{q}_i p_i - L(q_i, \dot{q}_i, q^0)$$

and represents the total energy of the system.

For the quantization of the Klein-Gordon field we consider in the following always a complex field $\Phi(R,t)$ as well as its complex conjugate field $\Phi^*(R,t)$ as independent field functions. In analogy to the classical Lagrangian for a noninteracting particle system, $L = T$ (kinetic energy), we construct a Lagrangian of the system as

$$L = \int d^3r \, \mathcal{L}(r, t) = \int d^3r \, \mathcal{L}(x)$$

where the Lagrangian density satisfies the Euler-Lagrange equations of motions

$$\partial^\mu \left[ \frac{\partial \mathcal{L}}{\partial (\partial^\mu \Phi^*)} \right] = \frac{\partial \mathcal{L}}{\partial \Phi^*}, \quad \partial^\mu \left[ \frac{\partial \mathcal{L}}{\partial (\partial^\mu \Phi)} \right] = \frac{\partial \mathcal{L}}{\partial \Phi}$$

such that the Euler-Lagrange equations of motion just give the Klein-Gordon equation (12) and its complex conjugate.
Quantization

For the Klein-Gordon field, the Lagrangian density then reads:

\[ \mathcal{L}(x) = [\partial_\mu \Phi^*(x)][\partial^\mu \Phi(x)] - m^2 \Phi^*(x)\Phi(x) \quad (26) \]

Canonical conjugate fields to \( \Phi(x) \) and \( \Phi^*(x) \) are defined in analogy to eq. (19):

\[ \pi(x) = \frac{\partial \mathcal{L}}{\partial (\partial^0 \Phi)} = \partial_0 \Phi^* = \dot{\Phi}^* \quad \pi^*(x) = \frac{\partial \mathcal{L}}{\partial (\partial^0 \Phi^*)} = \partial_0 \Phi = \dot{\Phi}. \quad (27) \]

We now consider the \( \Phi \) and \( \pi \) fields as operator valued space-time functions (field operators), where \( \Phi^\dagger \) and \( \pi^\dagger \) are the Hermitian adjoint field operators, and require similar to (22) the canonical commutation relations at the same time:

\[ [\Phi(r, t), \pi(r', t)] = i\delta^3(r - r'), \quad [\Phi^\dagger(r, t), \pi^\dagger(r', t)] = i\delta^3(r - r') \quad (28) \]

or

\[ \delta(r^0 - r'^0)[\Phi(r), \pi(r')] = i\delta^4(r - r') \quad (29) \]

All other commutators should vanish identically! The singular nature of these commutation relations shows that the field operators themselves have a singular space-time behavior, i.e. are operator valued distributions, and products of such operators must be handled computationally with caution.
The challenge is to find operator solutions of the Klein-Gordon equation (12) which satisfy eq. (28). In analogy to the Lagrange density (24), the hamiltonian is

\[ H = \int d^3r \, \mathcal{H}(r, t) \]  

with the **hamiltonian density**

\[ \mathcal{H}(x) = \pi(\partial^0 \Phi) + (\partial^0 \Phi^\dagger)\pi^\dagger - \mathcal{L}(x) = (\partial_0 \Phi^\dagger)(\partial^0 \Phi) + \pi \pi^\dagger - \mathcal{L}(x) \]  

or the **Hamiltonian density operator** of the field system reads:

\[ \mathcal{H} = \pi \pi^\dagger + (\nabla \Phi^\dagger) \cdot (\nabla \Phi) + m^2 \Phi^\dagger \Phi \]  

The interpretation of \( H \) follows from

\[ [\Phi(r, t), H(t)] = \int d^3r' \, [\Phi(r, t), \mathcal{H}(r', t)] = \int d^3r' \, [\Phi(r, t), \pi(r', t)]\pi^\dagger(r', t) = i \int d^3r' \, \pi^\dagger(r', t)\delta^3(r - r') = i\pi^\dagger(r, t) = i\partial^0 \Phi(r, t) \]  

and the **equation of motion**:

\[ [\pi(x), H(t)] = i\partial^0 \pi(x) \quad (\equiv i(\nabla^2 - m^2)\Phi^\dagger), \]
Quantization

For each operator $F$, which is a polynomial in the field operators $\Phi^+, \pi^+, \Phi, \pi$ we get:

$$i\partial^0 F = [F, H]$$  \hspace{1cm} (35)

and in particular

$$\partial^0 H = -i[H, H] = 0$$

i.e. the time independence of $H$ for a closed system (without interactions with an environment).

Analogously, for the $3$-vector operator (with convariant components $k=1,2,3$)

$$P^k = \int d^3r \left( \pi^\dagger \partial^k \Phi^\dagger + \pi \partial^k \Phi \right)$$  \hspace{1cm} (36)

we get

$$[P(t), \Phi(r, t)] = i\nabla \Phi(x), \quad [P(t), \pi(r, t)] = i\nabla \pi(x)$$  \hspace{1cm} (37)

$$[H, P] = 0$$  \hspace{1cm} (38)

One can now construct the $4$-vector operator $P$ such that

$$P = (H, P) \quad \text{with} \quad (P^0 = P_0 = H)$$  \hspace{1cm} (39)

$$[P^\mu, P^\nu] = 0 \quad (\nu, \mu = 0, 1, 2, 3)$$  \hspace{1cm} (40)

$\Rightarrow$ the space-time vector operator $P$ and an arbitrary operator $F$ follow

$$[F(x), P^\mu] = i\partial^\mu F(x)$$  \hspace{1cm} (41)

giving the space-time evolution of the operator $F$. 
Introduce the **annihilation operators** $a(q), b(q)$ and the **creation operators** $a^+(q), b^+(q)$ describing the annihilation and creation of states with 3-momentum $q$ (and positive and negative energy $\omega_q$).

The **solution of the Klein-Gordon equation** (12) can be expressed (in analogy to (9)) as

$$
\Phi(x) = \int \frac{d^3q}{2\omega_q} \left[ a(q)f_q(x) + b^+(q)f_q^*(x) \right],
$$

$$
\Phi^\dagger(x) = \int \frac{d^3q}{2\omega_q} \left[ a^+(q)f_q^*(x) + b(q)f_q(x) \right]
$$

**Using the orthonormalization relation** for the plane waves (13) one gets

$$
a(q) = i \int d^3r \left[ f_q^*(x) \partial^0 \Phi(x) - \partial^0 f_q^* (x) \Phi(x) \right] = (f_q, \Phi),
$$

$$
b(q) = i \int d^3r \left[ f_q^*(x) \partial^0 \Phi^\dagger(x) - \partial^0 f_q^*(x) \Phi^\dagger(x) \right] = (f_q, \Phi^\dagger),
$$

$$
b^+(q) = i \int d^3r \left[ f_q(x) \partial^0 \Phi(x) - \partial^0 f_q(x) \Phi(x) \right] = -(f_q^*, \Phi),
$$

$$
a^+(q) = i \int d^3r \left[ f_q(x) \partial^0 \Phi^\dagger(x) - \partial^0 f_q(x) \Phi^\dagger(x) \right] = -(f_q^*, \Phi^\dagger).\]
Using the commutation relation (28), and eqs. (44) , (13) \( \rightarrow \) for equal times \( x_0=y_0 \)

\[
\left[ a(q), a^\dagger(q') \right] = \int d^3x \int d^3y \left[ f_q^*(x) \partial_0^0 \Phi(x) - \partial_x^0 f_q^*(x) \Phi(x), f_{q'}(y) \partial_y^0 \Phi^\dagger(y) - \partial_y^0 f_{q'}(y) \Phi^\dagger(y) \right]_{y_0=x_0}
\]

\[
= \int d^3x \int d^3y \left\{ -f_q^*(x) \dot{f}_{q'}(y) \left[ \Phi(x), \Phi^\dagger(y) \right]_{y_0=x_0} - \dot{f}_q^*(x) f_{q'}(y) \left[ \Phi(x), \Phi^\dagger(y) \right]_{y_0=x_0} + \cdots \right\}
\]

\[
= i \int d^3x \left[ f_q^*(x) \dot{f}_{q'}(x) - \dot{f}_q^*(x) f_{q'}(x) \right] = (f_q, f_{q'}) = 2\omega_q \delta^3(q - q') \quad (45)
\]

In the same way one obtains:

\[
\left[ b(q), b^\dagger(q') \right] = 2\omega_q \delta^3(q - q') \quad (46)
\]

For all others combinations of \( a(q), b(q), a^+ (q), b^+ (q) \) the commutator vanishes !

Now consider the canonicelly conjugate fields using (42):

\[
\pi(x) = \partial_0 \Phi^\dagger = \int \frac{d^3q}{2\omega_q} \left[ -i\omega_q b(q) f_q(x) + i\omega_q a^\dagger(q) f_q^*(x) \right] \quad (47)
\]

Due to the orthogonality of plane waves, e.g. for the purely spatial integration we get

\[
\int d^3r f_q(x) f_q^*(x) = \delta^3(q - q'), \quad \int d^3r f_{q'}(x) f_q(x) = \delta^3(q + q') \exp(-2i\omega_q t)
\]
Particle-number representation

Accounting that $\omega_{-q} = \omega_q$ and after some transformations we obtain:

\[
H = \int \frac{d^3q}{2\omega_q} \left\{ \left( \omega_q^2 + q^2 + m^2 \right) [a^\dagger(q)a(q) + b(q)b^\dagger(q)] + \left( -\omega_q^2 + q^2 + m^2 \right) [a^\dagger(q)b^\dagger(-q) \exp(2i\omega_q t)] + b(q)a(-q) \exp(-2i\omega_q t) \right\}.
\] (48)

Using the “on-shell” condition: $\omega_q^2 = m^2 + q^2$

we obtain the classical Hamiltonian

\[
H = \int \frac{d^3q}{2\omega_q} [\omega_q a^\dagger(q)a(q) + \omega_q b(q)b^\dagger(q)].
\] (49)

Via the commutation relations it becomes apparent (see below) that $a(q)$

annihilates quanta of momentum $q$ whereas $a^\dagger(q)$ creates such quanta.

The same holds for the $b(q), b^\dagger(q)$ as seen from the following energy balance:
If $|E\rangle$ is an eigenstate of $H$ with eigenenergy $E$, then

$$H(a^\dagger(q)|E\rangle) = a^\dagger(q)(H|E\rangle) + \left[H, a^\dagger(q)\right]|E\rangle = (E + \omega_q)a^\dagger(q)|E\rangle,$$  \hspace{1cm} (51)

Which means that $a^\dagger(q)|E\rangle$ is also eigenstate of $H$ with energy $(E + \omega_q)$ i.e. it increases the energy by $\omega_q$.

In analogy for the annihilation operator $a(q)$ the energy is decreased:

$$H(a(q)|E\rangle) = (E - \omega_q)a(q)|E\rangle$$ \hspace{1cm} (52)

This verifies the interpretation of the $a, a^+, b, b^+$ as annihilation and creation operators of scalar field quanta.
Ordering of the field operators

A basic postulate of quantum field theory is the existence of a unique state of lowest energy $E_0$ (which is then shifted to $E_0=0$). For the vacuum state $|0\rangle$ one thus requires the proper normalization:

$$\langle 0 | 0 \rangle = 1 \quad \text{and} \quad H |0\rangle = 0 \quad \text{(53)}$$

Since the energy of the vacuum state can not be lowered by any operation one has to require:

$$\forall q : \quad a(q)|0\rangle = 0, \quad b(q)|0\rangle = 0. \quad \text{(54)}$$

With the form of $H$ according to (48-49), however, the second condition of (53), i.e. $H |0\rangle = 0$, is not satisfied since the expectation value

$$\langle 0 | H | 0 \rangle = E_0 \rightarrow \infty \quad \text{(55)}$$

leads to a divergent integral, and thus to a physically meaningless (not measurable) result!

To get all the physical properties required (i.e. (53)), the order of the operators in the $b$-term of $H$ must be reversed!

(Recall that for the classical Hamiltonian density the order plays no role whereas the order of operators is essential in quantum mechanics!)
Normal ordering of operators

We therefore define the order of operators in $H$ as follows:

$$H = \int \frac{d^3 q}{2\omega_q} [\omega_q a^\dagger(q) a(q) + \omega_q b^\dagger(q) b(q)].$$  \hspace{1cm} (56)

which automatically satisfy the condition $\langle 0 | H | 0 \rangle = 0$.

Normal ordering

In quantum field theory a product of creation and annihilation operators is in normal order (also called Wick order) when all creation operators are left of all annihilation operators in the product.

The process of transferring a product into normal order is denoted as normal ordering (also called Wick ordering).

The terms antinormal order and antinormal ordering are analogously defined, where the annihilation operators are placed to the left of the creation operators.
Normal ordering

Example for bosons

1) Normal ordering: \( :b^+(q')\ b(q) := b^+(q')\ b(q) \)

2) Define \( :b(q)\ b^+(q') : \)

From the commutation relation (46) \( \left[ b(q), b^+(q') \right] = 2\omega_q \delta^3(q - q') \)

\( \Rightarrow \quad b(q)\ b^+(q') = b^+(q')\ b(q) + 2\omega_q \delta^3(q - q') \)

\( \Rightarrow \) Normal ordering: \( :b(q)\ b^+(q') := b^+(q')\ b(q) \)

Notation:

The \( : \ldots : \) denote normal ordering!
Creating single-particles out of the vacuum

The normal ordered Hamiltonian for the Klein-Gordon field is given by

\[ \mathcal{H}(x) =: \pi(x)\pi^\dagger(x) + [\nabla \Phi^\dagger(x)] \cdot [\nabla \Phi(x)] + m^2 \Phi^\dagger(x)\Phi(x) :. \] (57)

The states

\[ |q, a\rangle = a^\dagger(q)|0\rangle, \quad |q, b\rangle = b^\dagger(q)|0\rangle, \] (58)

are orthonormal as a result of the commutation relations (45)

\[ \langle q', i | q, j \rangle = \delta_{ij} 2\omega_q \delta^3(q' - q), \quad i, j = a, b, \] (59)

With the normal ordered H (56) these states have the properties

\[ H|q, i\rangle = \omega_q |q, i\rangle, \quad i = a, b. \] (60)

and represent a single-particle state on top of the vacuum.
Analogously, for the operator $P$ (36)

$$P^k = \int d^3r \left( \pi^+ \partial^k \Phi + \pi \partial^k \Phi^\dagger \right)$$

after normal ordering: $:\ldots:\$ one gets

$$P = \int \frac{d^3q}{2\omega_q} \left[ q a^\dagger(q)a(q) + q b^\dagger(q)b(q) \right]$$

(61)

and the commutation relations give:

$$[a^\dagger(q), P] = -q a^\dagger(q), \quad [a(q), P] = q a(q),$$

(62)

which implies that $a^\dagger, b^\dagger$ and $a, b$ increase the momentum value of a $P$-eigenstate to $q$ or decrease it by $q$. Analogous to (60) we get

$$P |q, i\rangle = q |q, i\rangle, \quad i = a, b.$$  

(63)

This is the interpretation of $a^\dagger, b^\dagger$ and $a, b$ as creation and annihilation operators of the 'quantum field' with momentum $q$ and energy $\omega_q$ (of mass $m$).

Many-body states are obtained by applying subsequently more $a^\dagger, b^\dagger$ on the vacuum state:

$$|\Psi\rangle = \frac{1}{\sqrt{m!n!}} a^\dagger(p_1)\ldots a^\dagger(p_m) b^\dagger(q_1)\ldots b^\dagger(q_n) |0\rangle$$

(64)

with some normalization factor $N$ which depends on the $q_i$ and $p_j$ and is not specified explicitly here.
The total energy of a many-body state then is:

\[ H |\Psi\rangle = \left( \sum_{i=1}^{m} \omega_{p_i} + \sum_{j=1}^{n} \omega_{q_j} \right) |\Psi\rangle, \quad P |\Psi\rangle = \left( \sum_{i=1}^{m} p_i + \sum_{j=1}^{n} q_j \right) |\Psi\rangle. \] (65)

Particle number densities are defined via:

\[ N_a(q) = \frac{1}{2\omega_q} a^\dagger(q) a(q) \quad \quad N_b(q) = \frac{1}{2\omega_q} b^\dagger(q) b(q) \] (66)

for \( a \)- and \( b \)-type particles which act as:

\[ N_a(q) |\Psi\rangle = \left[ \sum_{i=1}^{m} \delta^3(q - p_i) \right] |\Psi\rangle, \quad N_b(q) |\Psi\rangle = \left[ \sum_{j=1}^{n} \delta^3(q - q_j) \right] |\Psi\rangle; \] (67)

The total particle number operators for \( a \)- and \( b \)-type particles then read:

\[ \hat{N}_a = \int d^3q \ N_a(q) \quad \text{and} \quad \hat{N}_b = \int d^3q \ N_b(q) \] (68)
Vacuum matrix elements

This leads to:
\[ \hat{N}_a |\Psi\rangle = m |\Psi\rangle \quad \text{and} \quad \hat{N}_b |\Psi\rangle = n |\Psi\rangle. \] (69)

With the help of the particle density operators the **four-momentum** reads:
\[ P^\mu = \int \frac{d^3q}{(2\pi)^3} q^\mu [N_a(\mathbf{q}) + N_b(\mathbf{q})]_{q_0=\sqrt{\mathbf{q}^2+m^2}}. \] (70)

which multiplies the particle densities simply with the individual four-momentum

A **single-particle wavefunction** then can be defined via the complex matrix element where \( |\Xi\rangle \) is an arbitrary state in Hilbert space:
\[ \langle q, a | \Xi \rangle = \langle 0 | a(\mathbf{q}) | \Xi \rangle = f(q) \] (71)

which is considered as a function of \( q : f(q) \). Its space-time representation is given by Fourier transformation:
\[ \psi_a(x) = \frac{1}{(2\pi)^{3/2}} \int \frac{d^3q}{2\omega_q} \exp \left[-i(\omega_q x^0 - \mathbf{q} \cdot \mathbf{r})\right] \langle 0 | a(\mathbf{q}) | \Xi \rangle \] (72)

which corresponds to the standard single-particle wavefunction in quantum mechanics.
A Lorentz transformation (with a 4 x 4 matrix $\Lambda$) implies:

$$x'_{\mu} = \sum_{\nu=0}^{3} \Lambda_{\mu}^{\nu} x_{\nu} = \Lambda_{\mu}^{\nu} x_{\nu}$$  \hspace{1cm} (72)$$

The metric is invariant:

$$g_{\mu\nu} \Lambda_{\rho}^{\mu} \Lambda_{\sigma}^{\nu} = g_{\rho\sigma}$$

Additional space-time transformations then give:

$$x^{\mu} \rightarrow x'^{\mu} = x^{\mu} + a^{\mu}$$

where $a^{\mu}$ is a constant vector denoting the space-time transformation

The combined transformations = Poincare transformations:

$$x \rightarrow x' = \Lambda x + a \hspace{0.5cm} \text{or} \hspace{0.5cm} x'^{\mu} = \Lambda_{\nu}^{\mu} x^{\nu} + a^{\mu}$$  \hspace{1cm} (73)$$

These transformations have 6 parameters for ordinary Lorentz transformations (3 for rotations and 3 for Lorentz-boosts) and 4 parameters for space-time transformations.

! The invariance of physical systems with respect to Poincare transformations is a fundamental requirement for any theoretical approaches!
Discrete transformation properties of the fields

- Invariance of the equations under the space-reversal transformation:

\[ x = (t, r) \rightarrow x' = (t, -r) \]  \hspace{1cm} (74)

\[ \Phi'(x') = \eta \Phi(x) \quad \text{with} \quad |\eta| = 1 \]

\[ \begin{align*}
\Phi'(-r, t) &= \Phi(r, t) \quad - \text{Scalar} \\
\Phi'(-r, t) &= -\Phi(r, t) \quad - \text{Pseudoscalar}
\end{align*} \]  \hspace{1cm} (75)

Definition: Internal Parity of the field: \( \eta = \pm 1 \)

- Invariance of the Klein-Gordon equation under time-reversal transformation:

\[ x = (t, r) \rightarrow x' = (-t, r) \]  \hspace{1cm} (76)

since it is a differential equation of second order in \( t \).
To find out the difference between the $a$- and $b$-particles, we consider the quantization of (16) for the current operator:

$$ j^\mu(x) = i [\Phi^*(x) \partial^\mu \Phi(x) - \partial^\mu \Phi^*(x) \Phi(x)] $$

The resulting current operator $j^\mu$ - analogously to the expression (57) for $H$ – is the normal ordered quantity

$$ j^\mu = i : \Phi^\dagger \partial^\mu \Phi - \partial^\mu \Phi^\dagger \Phi : $$

which also fulfills the continuity equation

$$ \partial_\mu j^\mu = 0 $$

By normal ordering we achieve that the spatial integral of the 'time' component - total charge $Q$ –

$$ Q = \int d^3r \ j^0(x) = i \int d^3r : (\Phi^\dagger \dot{\Phi} - \dot{\Phi}^\dagger \Phi) : $$

- after conversion to creation and annihilation operators - has the form

$$ Q = \int d^3q \ [N_a(q) - N_b(q)] = \hat{N}_a - \hat{N}_b = Q^\dagger $$
Charge and charge conjugation

The action of $Q$ on the vacuum state - like $H$ in (53) - has the eigenvalue zero:

$$Q |0\rangle = 0$$  \hspace{1cm} (80)

From (79) we get the time independence of $Q$, i.e. $Q$ is a conserved quantity!

$$[H, Q] = 0$$  \hspace{1cm} (81)

$$[Q, a^\dagger(q)] = a^\dagger(q), \quad [Q, b^\dagger(q)] = -b^\dagger(q),$$

$$[Q, a(q)] = -a(q), \quad [Q, b(q)] = b(q).$$  \hspace{1cm} (82)

The action of $a^+(q)$ increases the 'total charge' by one unit, while the action of $b^+(q)$ reduces it by one unit.

Thus the many-body states (64) are also eigenstates of $Q$ with

$$Q |\Psi\rangle = (m - n) |\Psi\rangle$$  \hspace{1cm} (83)
Equations (80) - (83) show that the Q-eigenvalues have the same properties as the electric charge measured in units of $e$: they are integers, additive and zero for the vacuum.

The complex free Klein-Gordon field therefore has a charge-like quantum number!

In the case of $\pi$-mesons, the $\pi^+$ and $\pi^-$ mesons represent $a$- and $b$- particles of opposite electrical charge. The $\pi^0$ particles are charge neutral and therefore described by a real valued field.

There are other ‘charge like’ states as the two electrically neutral mesons $K^0$, $\bar{K}^0$ in the family of the K-mesons, which are characterized by different values of the hypercharge $Y$.

Particles, like the $a$- and $b$-particles of the Klein-Gordon field with the same space-time transformation behavior - with equal rest mass and spin - but opposite values in one or more charge-like quantum numbers are called antiparticles. Thus, $\pi^-$ is the antiparticle to $\pi^+$ and vice versa. Similarly, $K^0$, $\bar{K}^0$ are antiparticles to each other since they have opposite hypercharge $Y$. 