
We want a decomposition of the scalar field where the energy k^0 is positive and where the Klein-Gordon equation is explicitly fulfilled.

In the momentum space $\partial^2 + m^2$ becomes $k^2 - m^2$ and we know that plane waves are a solution. Thus, we choose as an arbitrary solution of the Klein-Gordon equation an expansion as a Fourier-integral over plane wave solutions as follows:

$$\Phi(x) = \int d^4k \frac{1}{(2\pi)^{3/2}} \delta(k^2 - m^2) \theta(k^0) [A(k)e^{-ikx} + A^\dagger e^{ikx}]$$

where $\theta(k^0) = 1$ for $k^0 > 0$ and zero otherwise, and A, A^\dagger are operator-valued Fourier coefficients.

This can be simplified as follows

$$\Phi(x) = \int d^3k [a(k)e_k + a^\dagger(k)e_k^*]$$

with ($w_k = \sqrt{\vec{k}^2 + m^2}$)

$$e_k = \frac{e^{-ikx}}{\sqrt{(2\pi^3)2w_k}} \quad A(k) = \sqrt{2w_k}a(k)$$

Since the field operators satisfy the above equal-time commutation relations, the Fourier coefficients must also satisfy them

$$[a(k), a^\dagger(k')] = \delta^3(\vec{k} - \vec{k}')$$

and

$$[a(k), a(k')] = [a^\dagger(k), a^\dagger(k')] = 0$$

To find the spectrum of states we have to calculate the eigenstates of the Hamiltonian.

The Hamiltonian is the conserved “charge” associated with time translations:

Invariance of a physical system under infinitesimal translations in space-time

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

implies the conservation law

$$\partial_{\mu} T^{\mu\nu}(x) = 0$$

with the energy-momentum tensor $T^{\mu\nu}$

$$T^{\mu\nu}(x) = \frac{\partial \mathcal{L}}{\partial(\partial_{\mu} \Phi)} \partial^{\nu} \Phi - g^{\mu\nu} \mathcal{L}$$

The four constants of motion ($\partial_t P^\nu = 0$)

$$P^\nu = \int d^3x T^{0\nu}(x)$$

are the total energy of the system $H = \int d^3x T^{00}$ and its momentum vector $P^i = \int d^3x T^{0i}$, $i = 1, 2, 3$.

Thus, the Hamiltonian for the Klein-Gordon field reads

$$\begin{aligned} H &= \frac{1}{2} \int d^3x [\Pi^2 + \partial_i \Phi \partial_i \Phi + m^2 \Phi^2] = \\ &= \frac{1}{2} \int d^3k \omega_k [a(k)a^\dagger(k) + a^\dagger(k)a(k)] \end{aligned}$$

The field $\Phi(x)$ can be interpreted as a superposition of harmonic oscillators where a and a^\dagger denote the annihilation and creation operators, respectively.

The ground (vacuum) state $|0\rangle$ is defined as $a(k)|0\rangle = 0$ (normalized to $\langle 0|0\rangle = 1$) and is an eigenstate of H with the eigenvalue $\frac{1}{2} \int d^3k \omega_k \delta^3(0)$, the so-called zero point energy.

All other energy eigenstates can be build by acting on the vacuum state with creation operators, i.e. $a^\dagger(k)a^\dagger(p)\dots|0\rangle$ is an eigenstate of H with energy $\omega_k + \omega_p + \dots$

Because of the presence of the zero point energy, the energy of the vacuum state is infinite. However, we can simply disregard this term, since infinite shifts in the Hamiltonian cannot be measured, i.e. only energy differences not absolute values are measureable.

The fact that the zero point energy can be dropped is taken into account by assuming that product of fields at the same point in space-time are always *normal (Wick) ordered*: all annihilation(creation) operators are moved to the right(left)

$$\frac{1}{2}(a^\dagger a + a a^\dagger) \rightarrow: \frac{1}{2}(a^\dagger a + a a^\dagger) : \equiv a^\dagger a$$

Interpretation of the eigenstates:

The total energy-momentum operator reads

$$P^\mu = \frac{1}{2} \int d^3k k^\mu a^\dagger(k)a(k)$$

From the commutation relations it follows

$$[P^\mu, a^\dagger] = k^\mu a^\dagger \Rightarrow P^\mu a^\dagger |0\rangle = k^\mu a^\dagger |0\rangle$$

i.e. the state $|k\rangle = a^\dagger |0\rangle$ is an energy-momentum eigenstate. The operator a^\dagger creates a quantum with momentum \vec{k} and energy $\omega_k = \sqrt{\vec{k}^2 + m^2}$. Thus, these excitations can be called particles, since they are discrete entities that have the proper relativistic energy-momentum relation. The energy and the norm $\langle k|k'\rangle = \delta^3(\vec{k} - \vec{k}')$ of the states are always positive.

The state

$$\Phi(x)|0\rangle = \int d^3k e^{-ikx} |k\rangle$$

can be interpreted as a linear superposition of single particle states that have well-defined momentum.

The field-particle duality now becomes evident:

$$\langle k|\Phi(x)|0 \rangle = \langle 0|a(k)\Phi(x)|0 \rangle = e^{ikx}$$

i.e. the field Φ (its negative frequency part) acting on the vacuum creates a particle at point x with continuous momentum spectrum and propagating as a plane wave (with positive energy).

The requirement of (micro) causality as expressed in form of equal-time commutation relations for the field operators leads to the Bose-characteristics of the Klein-Gordon field:

$$a^\dagger(k_1)a^\dagger(k_2)|0 \rangle = a^\dagger(k_2)a^\dagger(k_1)|0 \rangle$$

$$|k_1, k_2 \rangle = |k_2, k_1 \rangle$$