Canonical quantization of a free scalar field

Lagrangian, current, energy

If the equations of motion for the field—the Euler-Lagrange equations—are to be linear second order differential equations, the Lagrangian must be quadratic in terms of the field and must contain only the field itself and its first derivatives.

And it must also be a real Lorentz scalar.

For a complex scalar field ϕ these conditions allow basically only one possible Lagrangian,

$$\mathcal{L} = \partial_a \phi^* \partial^a \phi - m^2 \phi^* \phi \ , \tag{1}$$

where m is some constant, later to be identified with the mass of the field quantum.

The Euler-Lagrange equation of this Lagrangian is the so called *Klein-Gordon equation*,

$$\partial_a \partial^a \phi + m^2 \phi = 0 \ . \tag{2}$$

The conserved current is given as

$$\begin{aligned} j^a &\doteq -i\left(\frac{\partial \mathcal{L}}{\partial(\partial_a \phi)}\phi - \frac{\partial \mathcal{L}}{\partial(\partial_a \phi^*)}\phi^*\right) \\ &= i(\phi^* \partial^a \phi - \partial^a \phi^* \phi) \ . \end{aligned} \tag{3}$$

The energy density is given the time-time component of the energy-momentum tensor,

$$\begin{aligned} T_0^0 &\doteq \frac{\partial \mathcal{L}}{\partial(\partial_0 \phi)}\partial_0 \phi + \frac{\partial \mathcal{L}}{\partial(\partial_0 \phi^*)}\partial_0 \phi^* - \mathcal{L} \\ &= \partial_t \phi^* \partial_t \phi + \nabla\phi^* \nabla\phi + m^2 \phi^* \phi. \end{aligned} \tag{4}$$

Normal modes

Normal modes are orthogonal and normalized solutions of the field equation with a given boundary condition.

Normal modes make a complete basis. Any other solution of the field equations with the same boundary condition can be represented as a linear superposition of normal modes.

Plane waves, spherical waves or stationary waves are often chosen as normal modes.

In canonical quantization the normal modes become quanta of the field.

Plane wave solutions

Let us try to find a solution of the Klein-Gordon equation in the form of a plane wave,

$$\phi(x) = e^{-ikx} \ , \tag{5}$$

where $k^a \doteq \{\omega, \mathbf{k}\}$, $kx \doteq k_a x^a = \omega t - \mathbf{kr}$.

Substituting (5) into the Klein-Gordon equation (2) gives

$$k^2 = m^2 \ , \tag{6}$$

where $k^2 \doteq k_a k^a = \omega^2 - \mathbf{k}^2$. This equation is apparently the well known relativistic relation between energy, mass and momentum of a particle,

$$\omega^2 = m^2 + \mathbf{k}^2 \ . \tag{7}$$

Thus, a plane wave with an arbitrary wave-vector $\mathbf{k}$ is a solution to the Klein-Gordon equation (2) as long as the frequency ω satisfies the relation (7).

Note that a *complete* basis must include both positive-frequency solutions with

$$\omega = +\sqrt{m^2 + \mathbf{k}^2} \ , \tag{8}$$

and negative-frequency solutions with

$$\omega = -\sqrt{m^2 + \mathbf{k}^2} \ . \tag{9}$$

Periodic boundary condition

Let us assume that our field is contained in a box of length L, much larger that the typical length of the physical system under consideration. Then the boundary condition on the surface of the box should be of little importance. We can then choose the boundary condition to our liking, and we choose the *periodic boundary condition*,

$$\phi|_{x^i=L} = \phi|_{x^i=0} \ , \ i = 1, 2, 3 \, . \tag{10}$$

For plane-waves $e^{i\mathbf{kr}}$ this means that the wave-vector $\mathbf{k}$ has to be of the form

$$k_x = \frac{2\pi}{L} n_x \ , \ k_y = \frac{2\pi}{L} n_y \ , \ k_z = \frac{2\pi}{L} n_z \ , \tag{11}$$

where n_x, n_y, n_z are integer numbers.

With this boundary condition the plane-waves with different wave-vectors are orthogonal,

$$\int_V d^3x e^{-i\mathbf{k'x}} e^{i\mathbf{kx}} = V \delta_{\mathbf{k'k}} \ , \tag{12}$$

where $\delta_{\mathbf{k'k}}$ is the Kronecker delta-symbol. The volume V should vanish from all final expressions, therefore we can just as well put it equal unity from the very beginning.

Normalization of normal modes to unit charge

A normal mode can be normalized covariantly to a unit charge Q, where

$$Q(\phi) \doteq \int_V dV j^0 = \int dV i \left(\phi^* \partial_t \phi - \partial_t \phi^* \phi\right) \ . \tag{13}$$

Substituting e^{-ikx} into (13) gives the total charge of a plane wave,

$$Q(e^{-ikx}) = 2\omega \,. \tag{14}$$

Note that positive-frequency solutions have positive charge, while negative-frequency solutions have negative charge.

Thus, a complete basis of orthogonal and normalized solutions to the Klein-Gordon equation can be chosen as a set of positive-frequency, $\phi^+_{\mathbf{k}}$, and negative-frequency, $\phi^-_{\mathbf{k}}$, plane-wave normal modes

$$\phi^+_{\mathbf{k}} = \frac{1}{\sqrt{2\omega_{\mathbf{k}}}} e^{-ikx} \,,\ \phi^-_{\mathbf{k}} = \frac{1}{\sqrt{2\omega_{\mathbf{k}}}} e^{+ikx} \,. \tag{15}$$

where $k^a \doteq \{\omega_{\mathbf{k}}, \mathbf{k}\}$ and $\omega_{\mathbf{k}} \doteq +\sqrt{m^2 + \mathbf{k}^2}$ is the *positive* square root.

Normal mode representation

Any solution ϕ to the field equation can be represented as a superposition of the normal modes,

$$\phi(x) = \sum_{\mathbf{k}} \frac{1}{\sqrt{2\omega_{\mathbf{k}}}} \left(a_{\mathbf{k}} e^{-ikx} + b^*_{\mathbf{k}} e^{ikx} \right) \,, \tag{16}$$

where the expansion coefficients $a_{\mathbf{k}}$ and $b_{\mathbf{k}}$ are complex numbers (soon to become operators).

The Hamiltonian in the normal mode representation is equal

$$H \doteq \int dV T^0_0 = \sum_{\mathbf{k}} \omega_{\mathbf{k}} (a^*_{\mathbf{k}} a_{\mathbf{k}} + b_{\mathbf{k}} b^*_{\mathbf{k}}) \,, \tag{17}$$

and the charge is equal

$$Q \doteq \int dV j^0 = \sum_{\mathbf{k}} (a^*_{\mathbf{k}} a_{\mathbf{k}} - b_{\mathbf{k}} b^*_{\mathbf{k}}) \,. \tag{18}$$

Note that the positive and negative frequency modes have the same energy but opposite charges. Like particles and antiparticles.

Canonical quantization

Experiment shows that the energy E and charge Q of a system of noninteracting particles/antiparticles are given as

$$E = \sum_{\mathbf{k}} \omega_{\mathbf{k}} (n_{\mathbf{k}} + \bar{n}_{\mathbf{k}}) \,, \tag{19}$$

$$Q = \sum_{\mathbf{k}} (n_{\mathbf{k}} - \bar{n}_{\mathbf{k}}) \,, \tag{20}$$

where $n_{\mathbf{k}}$ ($\bar{n}_{\mathbf{k}}$) is the number of particles (antiparticles) with momentum $\mathbf{k}$, both numbers being non-negative integers.

Mathematically the number of particles must then be represented by an operator—a matrix—with non-negative integer eigenvalues, acting on some abstract space of states.

Generation-annihilation operators

Comparing (19) and (20) with (17) and (18) we must postulate that the object $a^*_{\mathbf{k}} a_{\mathbf{k}}$ must be the number of particles operator,

$$n_{\mathbf{k}} = a^\dagger_{\mathbf{k}} a_{\mathbf{k}} \,, \tag{21}$$

with nonnegative integer eigenvalues.

This can be fulfilled if $a^\dagger_{\mathbf{k}}$ and $a_{\mathbf{k}}$—and similarly $b^\dagger_{\mathbf{k}}$ and $b_{\mathbf{k}}$—are themselves operators (called *generation-annihilation operators*) either with commutation relations

$$\begin{aligned} a_{\mathbf{k}} a^\dagger_{\mathbf{k}'} - a^\dagger_{\mathbf{k}'} a_{\mathbf{k}} &= \delta_{\mathbf{k}\mathbf{k}'} \,, \\ b_{\mathbf{k}} b^\dagger_{\mathbf{k}'} - b^\dagger_{\mathbf{k}'} b_{\mathbf{k}} &= \delta_{\mathbf{k}\mathbf{k}'} \,, \end{aligned} \tag{22}$$

(all other commutators are equal zero); or with anti-commutation relations

$$\begin{aligned} a_{\mathbf{k}} a^\dagger_{\mathbf{k}'} + a^\dagger_{\mathbf{k}'} a_{\mathbf{k}} &= \delta_{\mathbf{k}\mathbf{k}'} \,, \\ b_{\mathbf{k}} b^\dagger_{\mathbf{k}'} + b^\dagger_{\mathbf{k}'} b_{\mathbf{k}} &= \delta_{\mathbf{k}\mathbf{k}'} \,, \end{aligned} \tag{23}$$

(all other anti-commutators are equal zero).

The commutation relations (22) lead to the number of particle operator with eigenvalues $n_{\mathbf{k}} \in \{0, 1, 2, \dots\}$. In other words, any number of particles can be in the same state. Such particles are called *bosons*.

With the anti-commutation relations (23) the number of particle operator has only two eigenvalues $n_{\mathbf{k}} \in \{0, 1\}$. That is, at most one particle can occupy a given state. These particles are called *fermions*.

Using the bosonic commutation relations (22) we can rewrite the scalar Hamiltonian (17) as

$$H = \sum_{\mathbf{k}} \omega_{\mathbf{k}} (a^\dagger_{\mathbf{k}} a_{\mathbf{k}} + b^\dagger_{\mathbf{k}} b_{\mathbf{k}}) + \sum_{\mathbf{k}} \omega_{\mathbf{k}} \,, \tag{24}$$

which exactly corresponds to (19) except for the last term – a diverging integral. However, this term contains no operators – it is simply a constant shift of zero-energy. Therefore it can be safely ignored.

Spin and statistics

Note that we could not use the anti-commutation relation (23) in the scalar Hamiltonian (17) since in this case it would take the form

$$H = \sum_{\mathbf{k}} \omega_{\mathbf{k}} (a^\dagger_{\mathbf{k}} a_{\mathbf{k}} - b^\dagger_{\mathbf{k}} b_{\mathbf{k}}) \,, \tag{25}$$

which is not positive defined.

Thus in a canonical field theory the relation between spin and statistics follows automatically from the positive definiteness of the energy.