Canonical quantization of a scalar field

Lagrangian, current, energy

If the equation of motion for the field (the Euler-Lagrange equation) is to be a linear second order differential equation, the Lagrangian must be quadratic in the field and 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).

The Euler-Lagrange equation is the the *Klein-Gordon equation*,

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

The conserved current is given as

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

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

$$\begin{aligned} T^0_0 &= \frac{\partial\mathcal{L}}{\partial(\partial_0\phi)}\partial_0\phi + \frac{\partial\mathcal{L}}{\partial(\partial_0\phi^*)}\partial_0\phi^* - \mathcal{L} \\ &= \partial_t\phi^*\partial_t\phi + \nabla\phi^*\nabla\phi + m^2\phi^*\phi. \end{aligned} \tag{4}$$

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.

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 $k^a = \{\omega, \mathbf{k}\}$, $kx \equiv k_a x^a = \omega t - \mathbf{kr}$. Substituting (5) into the Klein-Gordon equation (2) gives

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

where $k^2 \equiv k_a k^a = \omega^2 - \mathbf{k}^2$. 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 $\omega = +\sqrt{m^2 + \mathbf{k}^2}$ and negative-frequency solutions with $\omega = -\sqrt{m^2 + \mathbf{k}^2}$.

Periodic boundary conditions

Let us assume that our field is contained in a box of length L, much larger that the typical length of the system. Then the boundary condition on the surface of the box should be of no importance for the system. We can then choose the boundary condition to our liking, and we choose a *periodic boundary condition*,

$$\phi|_{x^i = L} = \phi|_{x^i = 0} \,,\; i = 1, 2, 3 \,. \tag{8}$$

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

$$k_x = \frac{2\pi}{L} n_x \,,\; k_y = \frac{2\pi}{L} n_y \,,\; k_z = \frac{2\pi}{L} n_z \,, \tag{9}$$

where n_x, n_y, n_z are integer numbers.

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

$$\int_V d^3x e^{-i\mathbf{k'x}} e^{i\mathbf{kx}} = V \delta_{\mathbf{k'k}} \,, \tag{10}$$

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

Normalization to unit charge

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

$$Q(\phi) = \int_V dV j^0 = \int dV i\left(\phi^*\partial_t\phi - \partial_t\phi^*\phi\right) \,. \tag{11}$$

Substituting e^{-ikx} into (11) gives the total charge of a plane wave,

$$Q(e^{-ikx}) = 2\omega \,. \tag{12}$$

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

$$\phi^+_{\mathbf{k}} = \frac{1}{\sqrt{2\omega_{\mathbf{k}}}} e^{-ikx},\ \phi^-_{\mathbf{k}} = \frac{1}{\sqrt{2\omega_{\mathbf{k}}}} e^{+ikx} . \qquad (13)$$

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

Energy and charge in normal mode representation

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

$$\phi(x) = \sum_{\mathbf{k}} \frac{1}{\sqrt{2\omega_{\mathbf{k}}}} \left(a_{\mathbf{k}} e^{-ikx} + b^*_{\mathbf{k}} e^{ikx} \right) , \qquad (14)$$

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

$$H = \int dV T^0_0 = \sum_{\mathbf{k}} \omega_{\mathbf{k}} (a^*_{\mathbf{k}} a_{\mathbf{k}} + b_{\mathbf{k}} b^*_{\mathbf{k}}) , \qquad (15)$$

and the charge is equal

$$Q = \int dV j^0 = \sum_{\mathbf{k}} (a^*_{\mathbf{k}} a_{\mathbf{k}} - b_{\mathbf{k}} b^*_{\mathbf{k}}) . \qquad (16)$$

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 of a system of noninteracting particles and antiparticles is given as

$$E = \sum_{\mathbf{k}} \omega_{\mathbf{k}} (n_{\mathbf{k}} + \bar{n}_{\mathbf{k}}) , \qquad (17)$$

while the total charge of such system is equal

$$Q = \sum_{\mathbf{k}} (n_{\mathbf{k}} - \bar{n}_{\mathbf{k}}) , \qquad (18)$$

where $n_{\mathbf{k}}$ is the number of particles, $\bar{n}_{\mathbf{k}}$ is the number of antiparticles with momentum $\mathbf{k}$, with 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.

Generation-annihilation operators

Comparing (17) and (18) with (15) and (16) we have got to postulate that the object $a^*_{\mathbf{k}} a_{\mathbf{k}}$ must be the number of particles operator, $n_{\mathbf{k}} = a^\dagger_{\mathbf{k}} a_{\mathbf{k}}$, 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

$$a_{\mathbf{k}} a^\dagger_{\mathbf{k}} - a^\dagger_{\mathbf{k}} a_{\mathbf{k}} = 1 , \qquad (19)$$

or with anti-commutation relations

$$a_{\mathbf{k}} a^\dagger_{\mathbf{k}} + a^\dagger_{\mathbf{k}} a_{\mathbf{k}} = 1 . \qquad (20)$$

The commutation relations (19) lead to the number of particle operator $n_{\mathbf{k}}$ with eigenvalues $n = 0, 1, 2, ...$ In other words any number of particles can be in the same state. Such particles are called bosons.

The anti-commutation relations (20) lead to the number of particle operator $n_{\mathbf{k}}$ with only two eigenvalues $n = 0, 1$. That is at most one particle can occupy a given state. These particles are called fermions.

Statistics

Apparently for the scalar field the commutation relation (19) has to be chosen, otherwise the Hamiltonian (15) will not be bounded from below. The scalar (spin-0) particles must then necessarily be bosons.

Exercises

1. Prove the orthogonality of normal modes with periodic boundary condition (10).
2. Given $aa^\dagger - a^\dagger a = 1$ ($aa^\dagger + a^\dagger a = 1$) find the eigenvalues of the $a^\dagger a$ operator.
3. For the Lagrangian $\mathcal{L} = \partial_a \phi^* \partial^a \phi - m^2 \phi^* \phi$ find the expressions for the energy-momentum tensor T^a_b and the conserved current density j^a.
4. Calculate the 4-momentum $P^a = \int dV T^{0a}$ and the conserved current j^a for a positive and negative frequency normal modes (13). Interpret the results.
5. Prove that different normal modes contribute to the energy (15) and the charge (16) independently (there are no interference terms in the sums).