Chapter 3

Canonical quantisation

We have already seen that the Klein–Gordon equation cannot be regarded as a single-particle equation. This is, of course, expected from a relativistic theory, since, as explained in the Introduction, the number of particles need not be conserved in such a theory. However, when we quantise the Klein–Gordon field ϕ, it is possible to come up with a consistent particle interpretation of it.

In this chapter, we shall examine the method of canonical or 'second' quantisation. This approach follows the usual treatment of quantum mechanics very closely. In particular, the field is regarded as an operator, which has to satisfy certain commutation relations. The main lesson we shall learn, is that a free field behaves like an infinite collection of quantum mechanical harmonic oscillators. This enables a field to potentially describe an infinite number of particles.

3.1 Classical mechanics and field theory

Before we begin, it is useful to recall that there are two approaches to solving problems in classical mechanics. The first is the Lagrangian approach, which we have already met in Chapter 2. In this case, the fundamental quantity of interest is the *action* S, defined in term of a Lagrangian L by

$$S = \int_{t_a}^{t_b} \mathrm{d}t \, L(x, \dot{x}, t) \,, \tag{3.1}$$

where the dot refers to total derivative with respect to time. To obtain the equation of motion, we have to vary S with respect to paths $x(t)$ that vanish at t_a and t_b. The equation of motion, or Euler–Lagrange equation, can be written as

$$\dot{p}_r = \frac{\partial L}{\partial x_r} \,, \qquad p_r = \frac{\partial L}{\partial \dot{x}_r} \,, \tag{3.2}$$

where r is a label of the coordinates and p_r is the momentum conjugate to x_r.

The other approach is the Hamiltonian approach, which is probably most familiar from quantum mechanics (but is also useful in classical mechanics). In this approach, we define the Hamiltonian by

$$H = p_r \dot{x}_r - L \,. \tag{3.3}$$

The equations of motion are

$$\dot{p}_r = -\frac{\partial H}{\partial x_r} \,, \qquad \dot{x}_r = \frac{\partial H}{\partial p_r} \,. \tag{3.4}$$

When we quantise the system, we impose the commutation relations:

$$[x_r, p_s] = i\delta_{rs} \,, \qquad [x_r, x_s] = 0 = [p_r, p_s] \,. \tag{3.5}$$

We now turn to classical fields. Perhaps the most familiar example of this is the electromagnetic field $A^\mu(x)$, which describes photons. Similarly, we may introduce fields for other particles, such as a scalar field $\phi(x^0, \mathbf{x})$ for a spin-0 particle such as the pion.

For a complete description at a certain time x^0, we need to know $\phi(x^0, \mathbf{x})$ for all $\mathbf{x}$. This means we require a continuous infinity of generalised coordinates:

$$x_r \to \phi(x^0, \mathbf{x}) \,, \tag{3.6}$$

i.e., the discrete label r is replaced by the continuous label $\mathbf{x}$. This is the correspondence between a particle and a field, which would be encountered repeatedly in this chapter.

To achieve relativistic invariance in the Lagrangian formalism, we rewrite the action (3.1) as

$$S = \int \mathrm{d}^4 x \, \mathcal{L} \,, \tag{3.7}$$

where $\mathcal{L}$ is the Lagrangian density that is related to the Lagrangian L by

$$L = \int \mathrm{d}^3x\,\mathcal{L}\,. \tag{3.8}$$

The Lagrangian density has to be a scalar function of the form $\mathcal{L} = \mathcal{L}(\phi, \partial\phi, x)$. However, since we would like it to be invariant under space-time transformations, we take instead $\mathcal{L} = \mathcal{L}(\phi, \partial\phi)$. This is valid for a closed system, but is not true in general when there are sources present as these would be located at specific points in space-time.

Now we perform a variation of ϕ that vanishes on the 3-dimensional integration boundary, which is usually taken to be at infinity. Requiring S to be stationary under this variation gives:

$$\begin{aligned} 0 &= \delta S \\ &= \int \mathrm{d}^4x \left\{ \frac{\partial\mathcal{L}}{\partial\phi}\delta\phi + \frac{\partial\mathcal{L}}{\partial(\partial_\mu\phi)}\delta(\partial_\mu\phi) \right\} \\ &= \int \mathrm{d}^4x \left\{ \frac{\partial\mathcal{L}}{\partial\phi}\delta\phi - \partial_\mu\left(\frac{\partial\mathcal{L}}{\partial(\partial_\mu\phi)}\right)\delta\phi + \partial_\mu\left(\frac{\partial\mathcal{L}}{\partial(\partial_\mu\phi)}\delta\phi\right) \right\}. \end{aligned} \tag{3.9}$$

The last term can be turned into a surface integral which vanishes. This yields the field equation (Euler–Lagrange equation):

$$\partial_\mu \frac{\partial\mathcal{L}}{\partial(\partial_\mu\phi)} = \frac{\partial\mathcal{L}}{\partial\phi}\,. \tag{3.10}$$

The Lagrangian formalism has the advantage that it is manifestly Lorentz covariant. However, in this chapter, we shall mainly be using the Hamiltonian formalism, which would make the link to quantum mechanics more direct. Starting with a Lagrangian density for the field ϕ, we define the *momentum conjugate* of ϕ to be

$$\pi(x) = \frac{\partial\mathcal{L}}{\partial\dot{\phi}(x)}\,. \tag{3.11}$$

The *Hamiltonian* is then given by

$$H = \int \mathrm{d}^3\mathbf{x}\,(\pi\dot{\phi} - \mathcal{L})\,, \tag{3.12}$$

in a way reminiscent of the situation in classical mechanics (3.3). Then the field equation can also be written as

$$\dot{\pi}(x) = -\frac{\delta H}{\delta\phi(x)}\,, \qquad \dot{\phi}(x) = \frac{\delta H}{\delta\pi(x)}\,, \tag{3.13}$$

where the functional derivative is defined by[1]

$$\frac{\delta\phi(x)}{\delta\phi(y)} = \delta^{(3)}(\mathbf{x}-\mathbf{y})\,. \tag{3.14}$$

Because the Hamiltonian formalism singles out a particular time, it is not obvious that the field equations obey special relativity.

Given a Lagrangian density, there is a tensor known as the *energy-momentum tensor* that can be defined as

$$T^{\mu\nu} = \partial^\mu\phi\frac{\partial\mathcal{L}}{\partial(\partial_\nu\phi)} - g^{\mu\nu}\mathcal{L}\,, \tag{3.15}$$

so that the Hamiltonian can be written as

$$H = \int \mathrm{d}^3\mathbf{x}\,T^{00}. \tag{3.16}$$

Since $\mathcal{L}$ does not explicitly depend on t, we have $\dot{H}=0$. Note that

$$\partial_\nu T^{\mu\nu} = \partial^\mu\phi\partial_\nu\frac{\partial\mathcal{L}}{\partial(\partial_\nu\phi)} + (\partial_\nu\partial^\mu\phi)\frac{\partial\mathcal{L}}{\partial(\partial_\nu\phi)} - \partial^\mu\mathcal{L}\,. \tag{3.17}$$

But

$$\partial^\mu\mathcal{L} = \frac{\partial\mathcal{L}}{\partial\phi}\partial^\mu\phi + \frac{\partial\mathcal{L}}{\partial(\partial_\nu\phi)}(\partial^\mu\partial_\nu\phi)\,. \tag{3.18}$$

Hence

$$\partial_\nu T^{\mu\nu} = 0\,, \tag{3.19}$$

from the field equation. From this it follows that

$$0 = \int \mathrm{d}^3\mathbf{x}\,\partial_\nu T^{\mu\nu} = \partial_0\int \mathrm{d}^3\mathbf{x}\,T^{\mu 0} + \int \mathrm{d}^3\mathbf{x}\,\partial_k T^{\mu k}. \tag{3.20}$$

By the divergence theorem, we may write the second term on the right-hand side as an integral over a surface which encloses the system, and so the second term is zero. Therefore $\dot{P}^k = 0$, where

$$P^k \equiv \int \mathrm{d}^3\mathbf{x}\,T^{k0}\,, \tag{3.21}$$

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[1] Note that the field equation, with this definition, is often written as

$$\frac{\delta S}{\delta\phi(x)} = 0\,.$$

is the '4-momentum' carried by the field. H is the zeroth component of P^k.

In general, an invariance property of $\mathcal{L}$ is equivalent to a conservation law. This is known as Nöther's theorem. Suppose

$$\mathcal{L} = \mathcal{L}(\phi_r, \partial\phi_r)\,, \qquad r = 1, 2, \ldots\,. \tag{3.22}$$

Let $\phi_r \to \phi_r + \delta\phi_r$ be a variation of the fields, so that

$$\begin{aligned} \delta\mathcal{L} &= \frac{\partial\mathcal{L}}{\partial\phi_r}\delta\phi_r + \frac{\partial\mathcal{L}}{\partial(\partial_\mu\phi_r)}\delta(\partial_\mu\phi_r) \\ &= \left(\frac{\partial\mathcal{L}}{\partial\phi_r} - \partial_\mu\frac{\partial\mathcal{L}}{\partial(\partial_\mu\phi_r)}\right)\delta\phi_r + \partial_\mu\left(\frac{\partial\mathcal{L}}{\partial(\partial_\mu\phi_r)}\delta\phi_r\right)\,. \end{aligned} \tag{3.23}$$

But the first term vanishes by the Euler–Lagrange equation (3.10). If $\mathcal{L}$ is invariant under this variation, then we require that $\partial_\mu j^\mu = 0$, where the *conserved current* is given by

$$j^\mu = \text{const}\,\frac{\partial\mathcal{L}}{\partial(\partial_\mu\phi_r)}\delta\phi_r\,. \tag{3.24}$$

The corresponding *charge* is

$$Q \equiv \int \mathrm{d}^3\mathbf{x}\, j^0, \tag{3.25}$$

which is constant in time.

3.2 Real scalar field

Perhaps the simplest example of a field theory is that of a real scalar field ϕ satisfying the Klein–Gordon equation. It can be checked that this equation can be derived from the Lagrangian (density):

$$\mathcal{L} = \tfrac{1}{2}\left\{\partial_\mu\phi\partial^\mu\phi - m^2\phi^2\right\}. \tag{3.26}$$

The momentum conjugate field to ϕ is then

$$\pi = \frac{\partial\mathcal{L}}{\partial\dot{\phi}} = \dot{\phi}\,,$$

from which we get the Hamiltonian

$$H = \int \mathrm{d}^3\mathbf{x}\,\left\{\tfrac{1}{2}\pi^2 + \tfrac{1}{2}(\nabla\phi)^2 + \tfrac{1}{2}m^2\phi^2\right\}. \tag{3.27}$$

Note that this expression is positive-definite, so we do not have any problems with negative energies. The canonical quantisation procedure is to regard ϕ and π as *operators*, satisfying the analogue of (3.5):

$$\begin{aligned}[\phi(t,\mathbf{x}),\pi(t,\mathbf{y})] &= i\delta^{(3)}(\mathbf{x}-\mathbf{y})\,,\\ [\phi(t,\mathbf{x}),\phi(t,\mathbf{y})] = 0 &= [\pi(t,\mathbf{x}),\pi(t,\mathbf{y})]\,,\end{aligned} \tag{3.28}$$

where $\delta^{(3)}$ is the three-dimensional Dirac delta function. These are known as the canonical or equal-time commutation relations, since they are defined at a particular instant of time.

We first find the most general solution to the Klein–Gordon equation. It turns out to be more convenient to work in momentum space. We write the Fourier transform of $\phi(x)$ as $\phi(k)$, where

$$\phi(x) = \int \frac{\mathrm{d}^4k}{(2\pi)^4}\mathrm{e}^{-ik\cdot x}\phi(k)\,, \tag{3.29}$$

and

$$\phi(k) = \int \mathrm{d}^4x\,\mathrm{e}^{ik\cdot x}\phi(x)\,. \tag{3.30}$$

Since ϕ is Hermitian: $\phi^\dagger(x) = \phi(x)$, we have $\phi^\dagger(k) = \phi(-k)$. The Klein–Gordon equation in momentum space is then, quite simply,

$$(k^2 - m^2)\phi(k) = 0\,. \tag{3.31}$$

A solution to this can be written as

$$\phi(k) = \begin{cases} 2\pi\delta(k^2-m^2)a(\mathbf{k}) & k^0 > 0,\\ 2\pi\delta(k^2-m^2)a^\dagger(-\mathbf{k}) & k^0 < 0,\end{cases} \tag{3.32}$$

where a and $a^\dagger$ are as yet arbitrary operators.

Now, note that we can write (3.29) as

$$\phi(x) = \int \frac{\mathrm{d}^4k}{(2\pi)^4}\{\phi(k)\mathrm{e}^{-ik\cdot x} + \phi(-k)\mathrm{e}^{ik\cdot x}\}\theta(k^0)\,, \tag{3.33}$$

where

$$\theta(x) = \begin{cases} 1 & x > 0,\\ 0 & x \le 0,\end{cases} \tag{3.34}$$

is the step-function. Suppose we introduce the notation $\omega_{\mathbf{k}} \equiv \sqrt{\mathbf{k}^2 + m^2}$ for the energy. Using properties of the Dirac delta function, in particular,

$$\delta(f(x)) = \sum_{\substack{x_i \\ f(x_i)=0}} \frac{\delta(x - x_i)}{|f'(x_i)|}, \tag{3.35}$$

we then have

$$\begin{aligned}
\frac{\mathrm{d}^4 k}{(2\pi)^4} 2\pi \delta(k^2 - m^2)\theta(k^0) &= \frac{\mathrm{d}^4 k}{(2\pi)^3} \delta[(k^0)^2 - \omega_{\mathbf{k}}{}^2]\theta(k^0) \\
&= \frac{\mathrm{d}^4 k}{(2\pi)^3} \delta[(k^0 + \omega_{\mathbf{k}})(k^0 - \omega_{\mathbf{k}})]\theta(k^0) \\
&= \frac{\mathrm{d}^4 k}{(2\pi)^3} \frac{1}{2k^0} [\delta(k^0 + \omega_{\mathbf{k}}) + \delta(k^0 - \omega_{\mathbf{k}})]\theta(k^0) \\
&= \frac{\mathrm{d}^3 \mathbf{k}}{(2\pi)^3} \frac{\mathrm{d}k^0}{2k^0} \delta(k^0 - \omega_{\mathbf{k}}) \\
&= \frac{\mathrm{d}^3 \mathbf{k}}{(2\pi)^3 2\omega_{\mathbf{k}}},
\end{aligned} \tag{3.36}$$

which is a more convenient way of expressing the measure, although it looks non-covariant. In writing the last line, it is understood that $k^0 = \omega_{\mathbf{k}}$. Using (3.32) and (3.36), (3.33) then becomes

$$\begin{aligned}
\phi(x) &= \int \frac{\mathrm{d}^3 \mathbf{k}}{(2\pi)^3 2\omega_{\mathbf{k}}} \{a(\mathbf{k})\mathrm{e}^{-ik\cdot x} + a^\dagger(\mathbf{k})\mathrm{e}^{ik\cdot x}\} \\
&\equiv \phi^{(+)}(x) + \phi^{(-)}(x),
\end{aligned} \tag{3.37}$$

in terms of a sum of positive- and negative-frequency modes. Thus, the free-field operator $\phi(x)$ can be thought of as a superposition of plane-wave solutions to the Klein–Gordon equation. a and $a^\dagger$ are operators, acting on the state vectors of a Hilbert space. We shall now find their commutation relations and construct this space of states.

Introduce the positive energy (frequency) solutions:

$$f_k(x) = \frac{1}{[(2\pi)^3 2\omega_{\mathbf{k}}]^{1/2}} \mathrm{e}^{-ik\cdot x}, \tag{3.38}$$

which form an orthonormal basis in the sense that

$$\int \mathrm{d}^3\mathbf{x}\, f_k^*(x) i\overleftrightarrow{\partial_0} f_{k'}(x) = \delta^{(3)}(\mathbf{k} - \mathbf{k}'), \tag{3.39}$$

where $\overleftrightarrow{\partial_0} \equiv \overrightarrow{\partial_0} - \overleftarrow{\partial_0}$. Now, in terms of f_k, (3.37) becomes

$$\phi(x) = \int \frac{\mathrm{d}^3 k}{[(2\pi)^3 2\omega_{\mathbf{k}}]^{1/2}} \{ f_k(x) a(\mathbf{k}) + f_k^*(x) a^\dagger(\mathbf{k}) \} . \tag{3.40}$$

We can then invert this using (3.39) to get

$$\begin{aligned} a(\mathbf{k}) &= \int \mathrm{d}^3\mathbf{x}\, [(2\pi)^3 2\omega_{\mathbf{k}}]^{1/2} f_k^*(x) i \overleftrightarrow{\partial_0} \phi(x) , \\ a^\dagger(\mathbf{k}') &= \int \mathrm{d}^3\mathbf{x}'\, [(2\pi)^3 2\omega_{\mathbf{k}'}]^{1/2} \phi(x') i \overleftrightarrow{\partial_0} f_{k'}(x') . \end{aligned} \tag{3.41}$$

Hence, their commutator is

$$\begin{aligned} [a(\mathbf{k}), a^\dagger(\mathbf{k}')] &= - \int \mathrm{d}^3\mathbf{x} \int \mathrm{d}^3\mathbf{x}'\, (2\pi)^3 \sqrt{4\omega_{\mathbf{k}}\omega_{\mathbf{k}'}} [f_k^*(x) \overleftrightarrow{\partial_0} \phi(x), \phi(x') \overleftrightarrow{\partial_0} f_{k'}(x')] \\ &= (2\pi)^3 \int \mathrm{d}^3\mathbf{x} \int \mathrm{d}^3\mathbf{x}'\, \sqrt{4\omega_{\mathbf{k}}\omega_{\mathbf{k}'}} f_k^*(x) \overleftrightarrow{\partial_0} f_{k'}(x') [\phi(x), \pi(x')] \\ &= (2\pi)^3 2\omega_{\mathbf{k}} \delta^{(3)}(\mathbf{k} - \mathbf{k}') , \end{aligned} \tag{3.42}$$

where we have used (3.28) and (3.39) to evaluate the integral. Similarly, it can be checked that

$$[a(\mathbf{k}), a(\mathbf{k}')] = 0 = [a^\dagger(\mathbf{k}), a^\dagger(\mathbf{k}')] . \tag{3.43}$$

Observe that (3.42) and (3.43) look almost the same as the commutation relations for the creation and annihilation operators of the quantum mechanical harmonic oscillator. To push this analogy further, we introduce the operator

$$N(\mathbf{k}) = a^\dagger(\mathbf{k}) a(\mathbf{k}) . \tag{3.44}$$

Since they mutually commute: $[N(\mathbf{k}), N(\mathbf{k}')] = 0$, the eigenstates of $N(\mathbf{k})$ can be used to form a basis of the state space. Let us denote its eigenvalues by $n(\mathbf{k})$, so that

$$N(\mathbf{k}) |n(\mathbf{k})\rangle = n(\mathbf{k}) |n(\mathbf{k})\rangle . \tag{3.45}$$

Now, because

$$[N(\mathbf{k}), a^\dagger(\mathbf{k})] = a^\dagger(\mathbf{k}) , \qquad [N(\mathbf{k}), a(\mathbf{k})] = -a(\mathbf{k}) , \tag{3.46}$$

we have

$$\begin{aligned} N(\mathbf{k}) a^\dagger(\mathbf{k}) |n(\mathbf{k})\rangle &= \{n(\mathbf{k}) + 1\} a^\dagger(\mathbf{k}) |n(\mathbf{k})\rangle , \\ N(\mathbf{k}) a(\mathbf{k}) |n(\mathbf{k})\rangle &= \{n(\mathbf{k}) - 1\} a(\mathbf{k}) |n(\mathbf{k})\rangle . \end{aligned} \tag{3.47}$$

This means that $a^\dagger(\mathbf{k})$ acting on the state $|n(\mathbf{k})\rangle$ raises its eigenvalue by one, while $a(\mathbf{k})$ reduces it by one. Furthermore, $N(\mathbf{k})$ is non-negative, since

$$0 \le (a(\mathbf{k})|n(\mathbf{k})\rangle)^\dagger(a(\mathbf{k})|n(\mathbf{k})\rangle) = \langle n(\mathbf{k})|a^\dagger(\mathbf{k})a(\mathbf{k})|n(\mathbf{k})\rangle = n(\mathbf{k})\langle n(\mathbf{k})|n(\mathbf{k})\rangle\,. \tag{3.48}$$

Define the ground state $|0\rangle$ such that

$$a(\mathbf{k})|0\rangle = 0\,, \tag{3.49}$$

for all $\mathbf{k}$. Using the properties derived above, we deduce that $N(\mathbf{k})$ is integer-valued and non-negative. It can, in fact, be identified as the operator corresponding to the number of particles with 3-momentum $\mathbf{k}$. The operators $a^\dagger(\mathbf{k})$ and $a(\mathbf{k})$ are nothing but the creation and annihilation operators for the field quanta.

The Hamiltonian (3.27) can be written in terms of a and $a^\dagger$, using (3.37), as

$$\begin{aligned}
H &= \tfrac{1}{2}\int \mathrm{d}^3\mathbf{x}\,\{(\partial_0\phi)^2 + \nabla\phi\cdot\nabla\phi + m^2\phi^2\} \\
&= \tfrac{1}{2}\int \mathrm{d}^3\mathbf{x}\int\frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3 2\omega_{\mathbf{k}}}\int\frac{\mathrm{d}^3\mathbf{k}'}{(2\pi)^3 2\omega_{\mathbf{k}'}} \\
&\quad \Big\{\big(-ik_0 a(\mathbf{k})\mathrm{e}^{-ik\cdot x} + ik_0 a^\dagger(\mathbf{k})\mathrm{e}^{ik\cdot x}\big)\big(-ik_0' a(\mathbf{k}')\mathrm{e}^{-ik'\cdot x} + ik_0' a^\dagger(\mathbf{k}')\mathrm{e}^{ik'\cdot x}\big) \\
&\quad + \big(i\mathbf{k}a(\mathbf{k})\mathrm{e}^{-ik\cdot x} - i\mathbf{k}a^\dagger(\mathbf{k})\mathrm{e}^{ik\cdot x}\big)\cdot\big(i\mathbf{k}'a(\mathbf{k}')\mathrm{e}^{-ik'\cdot x} - i\mathbf{k}'a^\dagger(\mathbf{k}')\mathrm{e}^{ik'\cdot x}\big) \\
&\quad + m^2\big(a(\mathbf{k})\mathrm{e}^{-ik\cdot x} + a^\dagger(\mathbf{k})\mathrm{e}^{ik\cdot x}\big)\big(a(\mathbf{k}')\mathrm{e}^{-ik'\cdot x} + a^\dagger(\mathbf{k}')\mathrm{e}^{ik'\cdot x}\big)\Big\} \\
&= \tfrac{1}{2}\int \mathrm{d}^3\mathbf{x}\int\frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3 2\omega_{\mathbf{k}}}\int\frac{\mathrm{d}^3\mathbf{k}'}{(2\pi)^3 2\omega_{\mathbf{k}'}}\Big\{\big(-k_0k_0' - \mathbf{k}\cdot\mathbf{k}' + m^2\big)a(\mathbf{k})a(\mathbf{k}')\mathrm{e}^{-i(k+k')\cdot x} \\
&\quad + \big(k_0k_0' + \mathbf{k}\cdot\mathbf{k}' + m^2\big)a(\mathbf{k})a^\dagger(\mathbf{k}')\mathrm{e}^{i(k'-k)\cdot x} \\
&\quad + \big(k_0k_0' + \mathbf{k}\cdot\mathbf{k}' + m^2\big)a^\dagger(\mathbf{k})a(\mathbf{k}')\mathrm{e}^{i(k-k')\cdot x} \\
&\quad + \big(-k_0k_0' - \mathbf{k}\cdot\mathbf{k}' + m^2\big)a^\dagger(\mathbf{k})a^\dagger(\mathbf{k}')\mathrm{e}^{i(k+k')\cdot x}\Big\} \\
&= \tfrac{1}{2}\int\frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3 2\omega_{\mathbf{k}}}\Big\{\frac{1}{2\omega_{-\mathbf{k}}}\big(-k_0^2 + \mathbf{k}^2 + m^2\big)a(\mathbf{k})a(-\mathbf{k})\mathrm{e}^{-2ik_0t} \\
&\quad + \frac{1}{2\omega_{\mathbf{k}}}\big(k_0^2 + \mathbf{k}^2 + m^2\big)a(\mathbf{k})a^\dagger(\mathbf{k}) + \frac{1}{2\omega_{\mathbf{k}}}\big(k_0^2 + \mathbf{k}^2 + m^2\big)a^\dagger(\mathbf{k})a(\mathbf{k}) \\
&\quad + \frac{1}{2\omega_{-\mathbf{k}}}\big(-k_0^2 + \mathbf{k}^2 + m^2\big)a^\dagger(\mathbf{k})a^\dagger(-\mathbf{k})\mathrm{e}^{2ik_0t}\Big\}\,.
\end{aligned}\tag{3.50}$$

But $k^2 = m^2$, so the first and fourth terms vanish. Also, we have from the mass-shell condition that $k_0^2 = \mathbf{k}^2 + m^2 = \omega_{\mathbf{k}}^2$. Hence,

$$H = \int\frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3 2\omega_{\mathbf{k}}}\,\frac{\omega_{\mathbf{k}}}{2}\{a^\dagger(\mathbf{k})a(\mathbf{k}) + a(\mathbf{k})a^\dagger(\mathbf{k})\}$$

$$= \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3 2\omega_{\mathbf{k}}} \, \omega_{\mathbf{k}} \{ N(\mathbf{k}) + \tfrac{1}{2} \} \,, \tag{3.51}$$

and similarly for the 3-momentum,

$$\mathbf{P} = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3 2\omega_{\mathbf{k}}} \, \mathbf{k} \{ N(\mathbf{k}) + \tfrac{1}{2} \} \,. \tag{3.52}$$

This completes the analogy with the quantum mechanical harmonic oscillator. It is now clear that a field can be regarded as an infinite number of harmonic oscillators, each labelled by the 3-momentum $\mathbf{k}$. This is a manifestation of the fact that a quantum field describes an *infinite* number of degrees of freedom, compared with the finite number described by quantum mechanical systems.

We now come to the first problem of quantum field theory. It is well-known that the harmonic oscillator has a non-zero ground state or vacuum energy, as is clear from the $\frac{1}{2}$ term in (3.51). Thus, a Klein–Gordon field, being composed of an infinite number of oscillators, will have an infinite ground state energy! To solve this problem, we assume that only energy differences, and not their absolute values, are measurable. One prescription to subtract off this infinite energy, is known as *normal ordering* and denoted by : :. This procedure involves reordering the operator factors, so that the positive frequency parts of ϕ are always to the right of the negative frequency parts:

$$: \phi\phi : \equiv \phi^{(+)}\phi^{(+)} + 2\phi^{(-)}\phi^{(+)} + \phi^{(-)}\phi^{(-)}. \tag{3.53}$$

Compare this to the usual case when

$$\phi\phi = \phi^{(+)}\phi^{(+)} + \phi^{(+)}\phi^{(-)} + \phi^{(-)}\phi^{(+)} + \phi^{(-)}\phi^{(-)}. \tag{3.54}$$

So, for example, consider normal-ordering the Hamiltonian:

$$H = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3 2\omega_{\mathbf{k}}} \frac{\omega_{\mathbf{k}}}{2} : a^\dagger(\mathbf{k})a(\mathbf{k}) + a(\mathbf{k})a^\dagger(\mathbf{k}) : \tag{3.55a}$$

$$= \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3 2\omega_{\mathbf{k}}} \, \omega_{\mathbf{k}} N(\mathbf{k}) \,, \tag{3.55b}$$

where we have interchanged the a and $a^\dagger$ in the second term on the right-hand side of (3.55a) (without using the commutation relations). Note that the $\frac{1}{2}$ has disappeared! The energy of the ground state is then $\langle 0|H|0\rangle = 0$, which is what we want.

The 4-momentum of the field is

$$P^\mu = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3 2\omega_\mathbf{k}}\, k^\mu a^\dagger(\mathbf{k}) a(\mathbf{k})\,, \tag{3.56}$$

It can be checked that

$$[P^\mu, \phi(x)] = -i\partial^\mu \phi(x)\,. \tag{3.57}$$

Hence, P^μ is the translation operator:

$$\phi(x+a) = \mathrm{e}^{ia\cdot P}\phi(x)\mathrm{e}^{-ia\cdot P}. \tag{3.58}$$

In particular, its time component is

$$\phi(t,\mathbf{x}) = \mathrm{e}^{iHt}\phi(0,\mathbf{x})\mathrm{e}^{-iHt}. \tag{3.59}$$

This is as expected for an operator in the Heisenberg picture.

Let us now turn to a discussion of the state space itself. We normalise ground state $|0\rangle$ to be $\langle 0|0\rangle = 1$, and define higher states by applying creation operators to it:

$$|\mathbf{k}_1, \mathbf{k}_2, \ldots, \mathbf{k}_n\rangle = a^\dagger(\mathbf{k}_1) a^\dagger(\mathbf{k}_2)\cdots a^\dagger(\mathbf{k}_n)|0\rangle\,. \tag{3.60}$$

Since $a^\dagger$ commute with one another (3.43), the states are symmetric, e.g., $|\mathbf{k}_1, \mathbf{k}_2\rangle = |\mathbf{k}_2, \mathbf{k}_1\rangle$. Hence, that particles we are dealing with are bosons: any number of particles can be in the same momentum state $|\mathbf{k}, \mathbf{k}, \ldots, \mathbf{k}\rangle$.

In particular, one-particle states are of the form $|\mathbf{k}\rangle = a^\dagger(\mathbf{k})|0\rangle$. The norm of this state is

$$\langle \mathbf{k}|\mathbf{k}'\rangle = \langle 0|[a(\mathbf{k}), a^\dagger(\mathbf{k}')]|0\rangle = (2\pi)^3 2\omega_\mathbf{k}\delta^{(3)}(\mathbf{k}-\mathbf{k}')\,, \tag{3.61}$$

from (3.42). This strange normalisation is typical of relativistic theories. It implies that the 'one'-particle state actually consists of $2k_0$ particles per unit volume. To see this, we have to construct the wave-function $\psi(x)$ corresponding to the operator $\phi(x)$ with momentum p:

$$\begin{aligned}
\psi(x) &= \langle 0|\phi(x)|p\rangle \\
&= \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3 2\omega_\mathbf{k}} \{\langle 0|a(\mathbf{k})|p\rangle \mathrm{e}^{-ik\cdot x} + \langle 0|a^\dagger(\mathbf{k})|p\rangle \mathrm{e}^{ik\cdot x}\} \\
&= \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3 2\omega_\mathbf{k}} \langle k|p\rangle \mathrm{e}^{-ik\cdot x} \\
&= \int \mathrm{d}^3\mathbf{k}\, \delta^{(3)}(k-p)\mathrm{e}^{-ik\cdot x} \\
&= \mathrm{e}^{-ip\cdot x},
\end{aligned} \tag{3.62}$$

where we have used $\langle 0|a(\mathbf{k}) = \langle k|$ and $\langle 0|a^\dagger(\mathbf{k}) = (a(\mathbf{k}|0\rangle)^\dagger = 0$ in the second line, and (3.61) in the third. Recall that the 4-vector probability current for the Klein–Gordon equation is

$$j_\mu = i\psi^* \overleftrightarrow{\partial}_\mu \psi = 2p_\mu \psi^* \psi \,. \tag{3.63}$$

Then, the number of particles per unit volume is

$$\int \mathrm{d}^3\mathbf{x}\, j_0 = \int \mathrm{d}^3\mathbf{x}\, 2p_0 \psi^* \psi = 2p_0 \,. \tag{3.64}$$

3.3 Complex scalar field

We now generalise to the case of a complex scalar field, which would entail some interesting new physics. It would be discovered below that this field describes *charged* particles, unlike the real scalar field which describes uncharged ones. But otherwise, the treatment of this case is similar to that of the previous section.

The Lagrangian that naturally generalises (3.26) is

$$\mathcal{L} = (\partial_\mu \phi^\dagger)(\partial^\mu \phi) - m^2 \phi^\dagger \phi \,. \tag{3.65}$$

We shall write

$$\phi = \phi_1 + i\phi_2 \,, \tag{3.66}$$

where ϕ_1 and ϕ_2 are hermitian. We now have two independent fields, both of which should be varied to make the action stationary. One way to do so is to vary ϕ and $\phi^\dagger$ independently, and temporarily forget that they are hermitian conjugates. The Euler–Lagrange equations give

$$(\partial^2 + m^2)\phi^\dagger = 0 \,, \qquad (\partial^2 + m^2)\phi = 0 \,, \tag{3.67}$$

when we vary ϕ and $\phi^\dagger$ respectively. The fields conjugate to ϕ and $\phi^\dagger$ are

$$\pi = \frac{\partial \mathcal{L}}{\partial \dot{\phi}} = \dot{\phi}^\dagger \,, \qquad \pi^\dagger = \frac{\partial \mathcal{L}}{\partial \dot{\phi}^\dagger} = \dot{\phi} \,, \tag{3.68}$$

from which we can read off the Hamiltonian

$$\begin{aligned} H &= \int \mathrm{d}^3\mathbf{x} \{\pi \dot{\phi} + \pi^\dagger \dot{\phi}^\dagger - \mathcal{L}\} \\ &= \int \mathrm{d}^3\mathbf{x} \{\pi^\dagger \pi + (\nabla \phi^\dagger)(\nabla \phi) + m^2 \phi^\dagger \phi\} \,. \end{aligned} \tag{3.69}$$

This is clearly positive-definite. The canonical commutation relations in this case are given by

$$\begin{aligned}[\phi(t,\mathbf{x}),\pi(t,\mathbf{y})] &= i\delta^{(3)}(\mathbf{x}-\mathbf{y})\,,\\ [\phi^\dagger(t,\mathbf{x}),\pi^\dagger(t,\mathbf{y})] &= i\delta^{(3)}(\mathbf{x}-\mathbf{y})\,,\end{aligned} \tag{3.70}$$

with all other commutators vanishing.

As before, the field-operators can be expanded as

$$\begin{aligned}\phi(x) &= \int \frac{\mathrm{d}^3k}{(2\pi)^3 2\omega_{\mathbf{k}}}\left\{a(\mathbf{k})\mathrm{e}^{-ik\cdot x} + b^\dagger(\mathbf{k})\mathrm{e}^{ik\cdot x}\right\},\\ \phi^\dagger(x) &= \int \frac{\mathrm{d}^3k}{(2\pi)^3 2\omega_{\mathbf{k}}}\left\{b(\mathbf{k})\mathrm{e}^{-ik\cdot x} + a^\dagger(\mathbf{k})\mathrm{e}^{ik\cdot x}\right\},\end{aligned} \tag{3.71}$$

where now we have two different operator-coefficients a and b to account for the fact that they are independent. It can be checked that the commutation relations (3.70) become

$$\begin{aligned}[a(\mathbf{k}),a^\dagger(\mathbf{k}')] &= (2\pi)^3 2\omega_{\mathbf{k}}\delta^{(3)}(\mathbf{k}-\mathbf{k}')\,,\\ [b(\mathbf{k}),b^\dagger(\mathbf{k}')] &= (2\pi)^3 2\omega_{\mathbf{k}}\delta^{(3)}(\mathbf{k}-\mathbf{k}')\,.\end{aligned} \tag{3.72}$$

Since there are no non-trivial commutation relations between a and b, they can be treated independently. Hence, we conclude that there are two different types of particles created by $a^\dagger$ and $b^\dagger$.

Let us denote by $N(\mathbf{k}) = a^\dagger(\mathbf{k})a(\mathbf{k})$ the number of particles corresponding to the operators a, $a^\dagger$, and by $\bar{N}(\mathbf{k}) = b^\dagger(\mathbf{k})b(\mathbf{k})$ the number of particles corresponding to b, $b^\dagger$. The Hamiltonian becomes, with normal ordering,

$$H = \int \frac{\mathrm{d}^3k}{(2\pi)^3 2\omega_{\mathbf{k}}}\omega_{\mathbf{k}}\left\{N(\mathbf{k}) + \bar{N}(\mathbf{k})\right\}. \tag{3.73}$$

Since both types of particles contribute equally to the Hamiltonian, they must have the same mass.

Notice that the Lagrangian $\mathcal{L}$ is invariant under the transformation

$$\phi \to \mathrm{e}^{i\alpha}\phi, \qquad \phi^\dagger \to \mathrm{e}^{-i\alpha}\phi^\dagger, \tag{3.74}$$

for a real constant α. Infinitesimally, these symmetry variations are $\delta\phi = i\alpha\phi$ and $\delta\phi^\dagger = -i\alpha\phi^\dagger$. Using (3.63), they give the conserved current $j^\mu = i\phi^\dagger\partial^\mu\phi$, which is hermitian.

This is like the Klein–Gordon case, but the difference is that now ϕ is an operator. With normal ordering, (3.25) becomes

$$
\begin{aligned}
Q &= \int \mathrm{d}^3\mathbf{x} \ : \phi^\dagger \frac{\partial \phi}{\partial t} - \frac{\partial \phi^\dagger}{\partial t}\phi : \\
&= \int \frac{\mathrm{d}^3 k}{(2\pi)^3 2\omega_{\mathbf{k}}} \{N(\mathbf{k}) - \bar{N}(\mathbf{k})\} \, .
\end{aligned}
\tag{3.75}
$$

This will be identified as the total-charge operator.

It follows from (3.75) that the a- and b-particles carry opposite charges $+q$ and $-q$ respectively. But apart from this, they are identical. This means that b is the anti-particle of a. Of course, the occurrence of anti-particles associated to particles of non-zero charge[2] is a fundamental property of relativistic theories.

An example of a spin-0 particle–anti-particle pair is the pi-mesons $\pi^\pm$. Taken together, they are described by a single complex scalar field. However, the neutral pi-meson π^0 is described by a real field.

3.4 Spinor field

The next case we shall consider is the spin-$\frac{1}{2}$ case, corresponding to a spinor field ψ described by the Dirac equation. The Lagrangian is

$$
\mathcal{L} = \bar{\psi}(i\gamma \cdot \overleftrightarrow{\partial} - m)\psi \, . \tag{3.76}
$$

Varying with respect to ψ and $\bar{\psi}$ give the Dirac equations for $\bar{\psi}$ and ψ:

$$
(i\gamma \cdot \partial + m)\bar{\psi} = 0 \, , \qquad (i\gamma \cdot \partial - m)\psi = 0 \, .
$$

The fields conjugate to ψ and $\bar{\psi}$ are

$$
\pi = \frac{\partial \mathcal{L}}{\partial \dot{\psi}} = \tfrac{1}{2} i \psi^\dagger, \qquad \pi^\dagger = \frac{\partial \mathcal{L}}{\partial \dot{\psi}^\dagger} = -\tfrac{1}{2} i \psi, \tag{3.77}
$$

and the Hamiltonian is

$$
\begin{aligned}
H &= \int \mathrm{d}^3\mathbf{x} \, \{\pi \dot{\psi} + \pi^\dagger \dot{\psi}^\dagger - \mathcal{L}\} \\
&= \int \mathrm{d}^3\mathbf{x} \, \tfrac{1}{2} \left\{ \psi^\dagger i \frac{\partial \psi}{\partial t} - i \frac{\partial \psi^\dagger}{\partial t}\psi \right\} .
\end{aligned}
\tag{3.78}
$$

---

[2] When $\phi^\dagger = \phi$, the particle is strictly neutral and is its own anti-particle.

Note that this is not positive-definite; it would only so after quantisation, as we shall see below.

Note that the Lagrangian $\mathcal{L}$ is invariant under the transformation $\psi \to e^{i\alpha}\psi$, $\bar{\psi} \to e^{-i\alpha}\bar{\psi}$, giving the conserved current $j^\mu = \bar{\psi}\gamma^\mu\psi$.

The general solution to the Dirac equation can be expanded in terms of plane-wave solutions as follows:

$$\begin{aligned}\psi(x) &= \int \frac{d^3\mathbf{k}}{(2\pi)^3 2\omega_{\mathbf{k}}} \sum_{r=1}^{2} \left\{ a_r(\mathbf{k}) u_r(\mathbf{k}) e^{-ik\cdot x} + b_r^\dagger(\mathbf{k}) v_r(\mathbf{k}) e^{ik\cdot x} \right\} , \\ \bar{\psi}(x) &= \int \frac{d^3\mathbf{k}}{(2\pi)^3 2\omega_{\mathbf{k}}} \sum_{r=1}^{2} \left\{ a_r^\dagger(\mathbf{k}) \bar{u}_r(\mathbf{k}) e^{ik\cdot x} + b_r(\mathbf{k}) \bar{v}_r(\mathbf{k}) e^{-ik\cdot x} \right\} .\end{aligned} \tag{3.79}$$

It is similar to the case of the charged scalar field, except that we have to also expand in terms of the spinor basis u_r and v_r introduced in (1.103) and (1.104). The momentum and charge of the field is then found to be

$$\begin{aligned}P^\mu &= \int \frac{d^3\mathbf{k}}{(2\pi)^3 2\omega_{\mathbf{k}}} k^\mu \sum_{r=1}^{2} \left\{ a_r^\dagger(\mathbf{k}) a_r(\mathbf{k}) - b_r(\mathbf{k}) b_r^\dagger(\mathbf{k}) \right\} , \\ Q &= \int \frac{d^3\mathbf{k}}{(2\pi)^3 2\omega_{\mathbf{k}}} \sum_{r=1}^{2} \left\{ a_r^\dagger(\mathbf{k}) a_r(\mathbf{k}) + b_r(\mathbf{k}) b_r^\dagger(\mathbf{k}) \right\} .\end{aligned} \tag{3.80}$$

In particular, the Hamiltonian $H = P^0$ does not appear to be positive-definite (while the charge does—there appears to be a mix-up between the two!). To rectify this, we have to impose *anti*-commutation relations instead of the usual commutation relations:

$$\begin{aligned}\{a_r(\mathbf{k}), a_s^\dagger(\mathbf{k}')\} &= (2\pi)^3 2\omega_{\mathbf{k}} \delta^{(3)}(\mathbf{k} - \mathbf{k}') \delta_{rs} , \\ \{b_r(\mathbf{k}), b_s^\dagger(\mathbf{k}')\} &= (2\pi)^3 2\omega_{\mathbf{k}} \delta^{(3)}(\mathbf{k} - \mathbf{k}') \delta_{rs} ,\end{aligned} \tag{3.81}$$

with all other anti-commutators vanishing. Hence, when we normal-order an operator, there has to be an additional change of sign for each interchange of Fermi-field operators. The normal-ordered Hamiltonian then becomes

$$H = \int \frac{d^3\mathbf{k}}{(2\pi)^3 2\omega_{\mathbf{k}}} k^0 \sum_{r=1}^{2} \left\{ a_r^\dagger(\mathbf{k}) a_r(\mathbf{k}) + b_r^\dagger(\mathbf{k}) b_r(\mathbf{k}) \right\} , \tag{3.82}$$

which is now positive-definite. Also, the normal-ordered total charge is

$$Q = \int \frac{d^3\mathbf{k}}{(2\pi)^3 2\omega_{\mathbf{k}}} \sum_{r=1}^{2} \left\{ a_r^\dagger(\mathbf{k}) a_r(\mathbf{k}) - b_r^\dagger(\mathbf{k}) b_r(\mathbf{k}) \right\} . \tag{3.83}$$

Like the previous case, we therefore deduce that $a^\dagger$ creates particles and $b^\dagger$ creates anti-particles of opposite charge. The vacuum is defined by

$$a_r(\mathbf{k})|0\rangle = 0 = b_r(\mathbf{k})|0\rangle\,, \tag{3.84}$$

for all r, $\mathbf{k}$. Spin-$\frac{1}{2}$ particles, say electrons, are created by applying $a^\dagger$ to it, while positrons are created by applying $b^\dagger$. This is a refinement of Dirac's description of anti-particles, since it does not assume the existence of the infinite Dirac sea.

Note that, from the anti-commutation relations (3.81),

$$|\mathbf{k}_1, r; \mathbf{k}_2, s\rangle = a_r^\dagger(\mathbf{k}_1)a_s^\dagger(\mathbf{k}_2)|0\rangle = -a_s^\dagger(\mathbf{k}_2)a_r^\dagger(\mathbf{k}_1)|0\rangle = -|\mathbf{k}_2, s; \mathbf{k}_1, r\rangle\,. \tag{3.85}$$

Hence, $|\mathbf{k}, r; \mathbf{k}, r\rangle = 0$, i.e., it is impossible to have two quanta of the Dirac field in the same state. This is, of course, Fermi–Dirac statistics at work.

3.5 Covariant commutation relations

The canonical commutation relations, that we have encountered, have the fundamental property of being defined for *equal* times. This means that a preferred time-slicing is singled out, and it is not clear if relativistic covariance is preserved, even though the Lagrangian formalism that we started off with is manifestly covariant. In this section, I shall introduce the so-called covariant commutation relations, which would address this problem.

Consider the commutator for the Klein–Gordon field at two arbitrary space-time points x and y:

$$[\phi(x), \phi(y)]\,. \tag{3.86}$$

This quantity is a Lorentz scalar, and so it must be invariant under Lorentz transformations. Let us evaluate this commutator.

Recall from (3.37) that ϕ can be written as a sum of positive- and negative-frequency parts. Because the a's commute between themselves, and similarly for the $a^\dagger$'s, we have

$$[\phi^{(+)}(x), \phi^{(+)}(y)] = 0 = [\phi^{(-)}(x), \phi^{(-)}(y)]\,. \tag{3.87}$$

However, the cross-term

$$[\phi^{(+)}(x), \phi^{(-)}(y)] = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3 2\omega_{\mathbf{k}}} \mathrm{e}^{-ik\cdot(x-y)} \,, \tag{3.88}$$

is non-vanishing. Hence,

$$\begin{aligned} [\phi(x), \phi(y)] &= [\phi^{(+)}(x), \phi^{(-)}(y)] + [\phi^{(-)}(x), \phi^{(+)}(y)] \\ &= \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3 2\omega_{\mathbf{k}}} \left\{ \mathrm{e}^{-ik\cdot(x-y)} - \mathrm{e}^{ik\cdot(x-y)} \right\} \\ &= i\triangle(x-y) \,, \end{aligned} \tag{3.89}$$

where we have defined

$$\triangle(x) = -i \int \frac{\mathrm{d}^4 k}{(2\pi)^4} 2\pi\delta(k^2 - m^2)\varepsilon(k^0)\mathrm{e}^{-ik\cdot x}, \tag{3.90}$$

and

$$\varepsilon(x) = \frac{x}{|x|} = \begin{cases} +1 & x > 0; \\ -1 & x < 0. \end{cases} \tag{3.91}$$

Let us consider some properties of the singular function $\triangle(x)$:

1 $\triangle(x)$ is invariant under Lorentz transformations $x \to x'$, since each factor in (3.90) is. In particular, $\varepsilon(k^0)$ is invariant since proper Lorentz transformations do not interchange future and past.

2 It satisfies the Klein–Gordon equation:

$$(\partial^2 + m^2)\triangle(x) = 0 \,. \tag{3.92}$$

3 When x is space-like,

$$\triangle(x) = 0 \,, \qquad \text{for } x^2 < 0 \,. \tag{3.93}$$

Thus, space-like separated $\phi(x)$ and $\phi(y)$ commute. This is an expression of causality: signals cannot travel faster than light, so for space-like x–y, the measurement of ϕ at x does not affect that at y.

Now, any two space-like separated points can be transformed into equal-time points by a Lorentz transformations. Hence, we have

$$\triangle(x) = 0 \,, \qquad \text{for } x^0 = 0 \,. \tag{3.94}$$

From this, we can recover the equal-time commutation relations (3.28).

4 We have

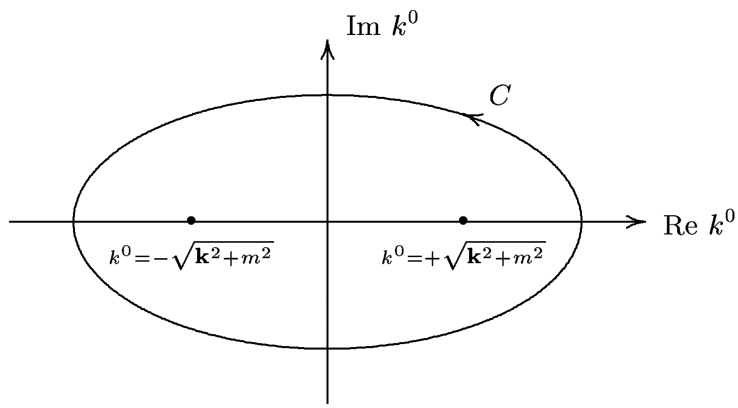
$$\frac{\partial}{\partial x^0}\triangle(x)\bigg|_{x^0=0} = -\delta^{(3)}(\mathbf{x})\,, \tag{3.95}$$

from which we recover the non-zero equal-time commutation relation $[\phi, \pi]$.

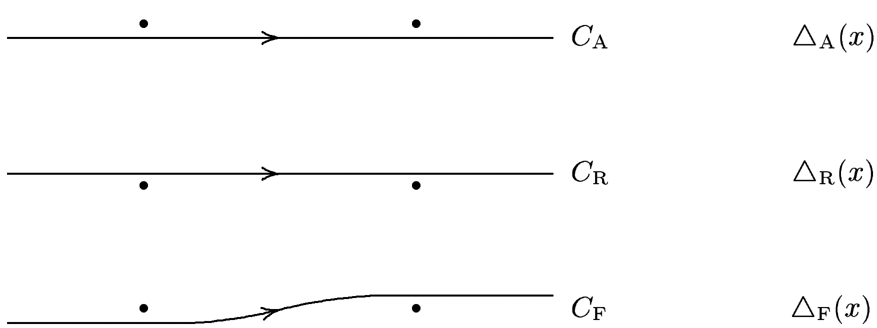
A useful way of representing $\triangle(x)$ is as a contour integral. Using (3.36), we have

$$\triangle(x) = -\oint_C \frac{\mathrm{d}^4 k}{(2\pi)^4}\frac{\mathrm{e}^{-ik\cdot x}}{k^2 - m^2}\,, \tag{3.96}$$

where C denotes the contour



followed by integration over real $\mathbf{k}$. Three other singular functions which are useful are $\triangle_{\rm A}$, $\triangle_{\rm R}$, and $\triangle_{\rm F}$, with the contours:



It can be verified that

$$(\partial^2 + m^2)G(x) = \delta(x)\,, \tag{3.97}$$

where $G = \triangle_{\rm A}$, $\triangle_{\rm R}$, or $\triangle_{\rm F}$ Thus, they are Green's functions of the Klein–Gordon equation. This means that

$$\Phi(x) \equiv \int \mathrm{d}^4y\, G(x-y)j(y)\,, \tag{3.98}$$

is a solution to the Klein–Gordon equation with a source: $(\partial^2 + m^2)\Phi(x) = j(x)$, subject to the appropriate boundary conditions.

Now, note that

$$\triangle_{\rm A}(x) = 0\,, \qquad \text{for } x^0 > 0\,, \tag{3.99}$$

since $\mathrm{e}^{-ik\cdot x}$ tends to zero on the infinite semi-circle in the lower-half plane. If we close the contour $C_{\rm A}$ using this semi-circle, we obtain a closed contour with no singularities inside. $\triangle_{\rm A}$ is known as the *advanced* Green's function. Similarly, if we use an infinite semi-circle in the upper-half plane, we arrive at the *retarded* Green's function

$$\triangle_{\rm R}(x) = 0\,, \qquad \text{for } x^0 < 0\,. \tag{3.100}$$

The case of the so-called *Feynman* Green's function is slightly more complicated. We close the contour using the lower-half semi-circle when $x^0 > 0$, and the upper-half semi-circle when $x^0 < 0$. Both contours would surround a pole, and we get

$$\triangle_{\rm F}(x) = \begin{cases} -i\int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3 2\omega_{\mathbf{k}}}\mathrm{e}^{-ik\cdot x} = -i[\phi^{(+)}(x), \phi^{(-)}(0)] & x^0 > 0; \\ -i\int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3 2\omega_{\mathbf{k}}}\mathrm{e}^{ik\cdot x} = -i[\phi^{(+)}(0), \phi^{(-)}(x)] & x^0 < 0, \end{cases} \tag{3.101}$$

where we have evaluated the contour integral using the method of residues, and used (3.88).

At this stage, it is useful to define the time-ordered product, denoted by T:

$$\begin{aligned} \mathrm{T}\,\phi(x)\phi(y) &= \begin{cases} \phi(x)\phi(y) & x^0 > y^0; \\ \phi(y)\phi(x) & y^0 > x^0. \end{cases} \\ &= \theta(x^0 - y^0)\phi(x)\phi(y) + \theta(y^0 - x^0)\phi(y)\phi(x)\,. \end{aligned} \tag{3.102}$$

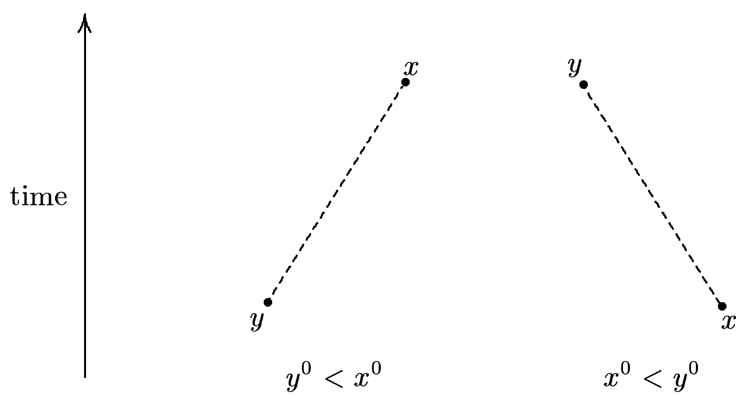
Taking the time-ordered product of a set of operators therefore ensures that operators defined at earlier times act first. Then, using (3.53), (3.54) and (3.101),

$$\mathrm{T}\,\phi(x)\phi(y) = :\phi(x)\phi(y): + i\triangle_{\rm F}(x-y)\,. \tag{3.103}$$

Taking the vacuum expectation value of this, and using the fact that in $:\phi\phi:$ all the annihilation operators are to the right of the creation operators, we have

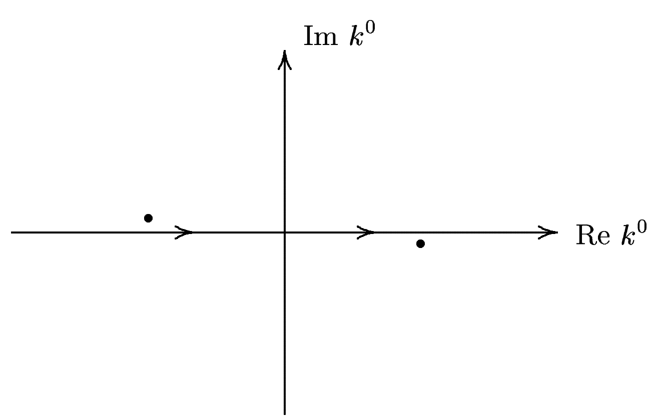
$$\langle 0|\mathrm{T}\,\phi(x)\phi(y)|0\rangle = i\triangle_{\mathrm{F}}(x-y)\,. \tag{3.104}$$

What is the physical interpretation of this vacuum expectation value? When $x^0 > y^0$, this expression can be thought of as representing a particle being created at y, travelling to x, and being annihilated at x. Similarly, when $y^0 > x^0$, a particle is created at x, propagates to y, and is absorbed.



For this reason, $\triangle_{\mathrm{F}}$ is also known as the Feynman propagator.

Now, instead of deforming the contour C_{F}, it is sometimes more convenient to move the poles an infinitesimal distance off the real axis with the redefinition $m^2 \to m^2 - i\epsilon$, where ϵ is real and positive:



Once this is done, the k^0 integration can be performed over the whole real axis, and we have

$$\triangle_{\mathrm{F}}(x) = \lim_{\epsilon \to 0^+} - \int \frac{\mathrm{d}^4 k}{(2\pi)^4} \frac{\mathrm{e}^{-ik \cdot x}}{k^2 - m^2 + i\epsilon} \,. \tag{3.105}$$

We shall also adopt Feynman's $i\epsilon$ prescription, where we do not write $\lim_{\epsilon \to 0^+}$ explicitly, but understand that it is present whenever $i\epsilon$ appears.

The generalisation to the complex scalar field is straightforward:

$$\langle 0 | \mathrm{T}\, \phi(x) \phi(y)^\dagger | 0 \rangle = i \triangle_{\mathrm{F}}(x - y) \,. \tag{3.106}$$

where $\triangle_{\mathrm{F}}$ is the same propagator as for the real scalar field.

For the Dirac field, we need to define

$$S(x) = (i\gamma \cdot \partial + m) \triangle(x) \,. \tag{3.107}$$

which is a 4×4 matrix satisfying the Dirac equation. Then,

$$\{\psi(x), \bar{\psi}(y)\} = iS(x - y) \,, \tag{3.108}$$

where

$$S(x) = - \oint_C \frac{\mathrm{d}^4 k}{(2\pi)^4} \frac{\gamma \cdot k + m}{k^2 - m^2} \mathrm{e}^{-ik \cdot x} = - \oint_C \frac{\mathrm{d}^4 k}{(2\pi)^4} \frac{\mathrm{e}^{-ik \cdot x}}{\gamma \cdot k - m} \,. \tag{3.109}$$

By choosing the contour C appropriately, we can define the analogue of the advanced, retarded and Feynman Green's functions S_{A}, S_{R} and S_{F}. In particular, we have

$$\langle 0 | \mathrm{T}\, \psi(x) \bar{\psi}(y) | 0 \rangle = i S_{\mathrm{F}}(x - y) \,, \tag{3.110}$$

where

$$S_{\mathrm{F}}(x) = - \int \frac{\mathrm{d}^4 k}{(2\pi)^4} \frac{\gamma \cdot k + m}{k^2 - m^2 + i\epsilon} \mathrm{e}^{-ik \cdot x} \,. \tag{3.111}$$

We are using Feynman's $i\epsilon$ prescription in writing this.

3.6 Electromagnetic field

We now consider the case of the spin-1 electromagnetic field. This is again similar to the previous cases, but now there is the added complication of so-called gauge invariance.

The Lagrangian for the electromagnetic field A_μ is

$$\mathcal{L} = -\tfrac{1}{4} F_{\mu\nu} F^{\mu\nu} , \tag{3.112}$$

where $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$. It looks quite different from those we have already encountered, but since it involves two derivatives, it is a kinetic term for A^μ. The Euler–Lagrange equation in this case is

$$\frac{\partial \mathcal{L}}{\partial A_\mu} - \partial_\nu \left(\frac{\partial \mathcal{L}}{\partial(\partial_\nu A_\mu)} \right) = 0 , \tag{3.113}$$

which reduces to

$$\partial_\mu F^{\mu\nu} = 0 , \tag{3.114}$$

i.e., Maxwell's equations! (3.114) can be rewritten in terms of A_μ as

$$\Box A^\nu - \partial^\nu (\partial_\mu A^\mu) = 0 . \tag{3.115}$$

Now, for a given electromagnetic field, A_μ is not unique. The gauge transformation

$$A_\mu \to A_\mu + \partial_\mu \Lambda , \tag{3.116}$$

leaves $F_{\mu\nu}$, and hence any physically measurable quantity, unchanged. We can therefore 'fix' the gauge, by say, choosing Λ to satisfy $\Box\Lambda = -\partial_\mu A^\mu$. In this case, we obtain

$$\partial_\mu A^\mu = 0 , \tag{3.117}$$

which is called the Lorentz gauge condition. It reduces the number of independent components of A_μ from four to three. However, A_μ is still not unique because we can still perform a gauge transformation (3.116) such that $\Box\Lambda = 0$. One way to address this, is to impose the additional constraint

$$A_0 = 0 , \tag{3.118}$$

known as the Coulomb gauge. With this condition, there are only two independent components of A^μ left, both of which are physical and cannot be gauged away. They correspond to the two transverse degrees of freedom of a photon.

The Coulomb gauge (3.118) gauge however, has the disadvantage that it is not a Lorentz invariant condition. Nevertheless, we can still carry out the canonical quantisation procedure, and it is quite similar to the case of the Klein–Gordon or Dirac field treated above. In this section, we shall follow a different quantisation procedure which is *covariant*, known as *Gupta–Bleuler quantisation*. In this case, we impose the Lorentz gauge but not the Coulomb one.

The Lorentz gauge (3.117) implies the field equation

$$\partial^2 A^\mu = 0\,, \tag{3.119}$$

which can be thought of as four massless Klein–Gordon equations, one for each component of μ. A Lagrangian which when varied gives (3.119) is

$$\mathcal{L} = -\tfrac{1}{2}(\partial_\mu A_\nu)(\partial^\mu A^\nu)\,. \tag{3.120}$$

The general solution to the field equation can then be expanded in terms of plane-waves as

$$A_\mu(x) = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3 2\omega_{\mathbf{k}}} \sum_{\lambda=0}^{3} \varepsilon_\mu^{(\lambda)}(k)\big\{a^{(\lambda)}(\mathbf{k})\mathrm{e}^{-ik\cdot x} + a^{(\lambda)\dagger}(\mathbf{k})\mathrm{e}^{ik\cdot x}\big\}\,, \tag{3.121}$$

where the coefficients $\varepsilon_\mu^{(\lambda)}$ are the polarisation vectors, which obey the normalisation

$$\varepsilon^{(\lambda)}\cdot\varepsilon^{(\lambda')} = g^{\lambda\lambda'}. \tag{3.122}$$

We assume, for simplicity, that the photon is moving along the third axis. Then, its 4-momentum vector is $k^\mu = (k, 0, 0, k)$, and the polarisation vectors can be taken to be

$$\varepsilon^{(0)} = \begin{pmatrix}1\\0\\0\\0\end{pmatrix}, \qquad \varepsilon^{(1)} = \begin{pmatrix}0\\1\\0\\0\end{pmatrix}, \qquad \varepsilon^{(2)} = \begin{pmatrix}0\\0\\1\\0\end{pmatrix}, \qquad \varepsilon^{(3)} = \begin{pmatrix}0\\0\\0\\1\end{pmatrix}. \tag{3.123}$$

Note that $k\cdot\varepsilon^{(1)} = 0 = k\cdot\varepsilon^{(2)}$, i.e., $\varepsilon^{(1)}$ and $\varepsilon^{(2)}$ are transverse to the direction of motion. Photons with polarisation $\varepsilon^{(0)}$ are known as scalar photons; with polarisation $\varepsilon^{(3)}$, longitudinal photons; and with polarisation $\varepsilon^{(1)}$ or $\varepsilon^{(2)}$, transverse photons. As mentioned above, only the two latter ones are physical.

The covariant quantisation procedure results in

$$[A^\mu(x), A^\nu(y)] = -ig^{\mu\nu}D(x-y)\,, \tag{3.124}$$

where the propagator is given in terms of (3.90) by

$$D(x) = \triangle(x)\big|_{m=0}\,. \tag{3.125}$$

This is almost identical to the Klein–Gordon case, except for an extra minus sign which is present because the spatial components of the metric $g_{\mu\nu}$ are -1. The corresponding photon creation and annihilation operators then satisfy the commutation relation

$$[a^{(\lambda)}(\mathbf{k}), a^{(\lambda')\dagger}(\mathbf{k}')] = -g^{\lambda\lambda'}(2\pi)^3 2\omega_{\mathbf{k}}\delta^{(3)}(\mathbf{k}-\mathbf{k}')\,, \tag{3.126}$$

with all other commutators vanishing.

The price of covariance, is that the $\lambda = \lambda' = 0$ commutation relation has the wrong sign. In particular, this means that $a^{(0)\dagger}(\mathbf{k})|0\rangle$ has negative norm:

$$\langle 0|a^{(0)}(\mathbf{k})a^{(0)\dagger}(\mathbf{k})|0\rangle = \langle 0|[a^{(0)}(\mathbf{k}), a^{(0)\dagger}(\mathbf{k})]|0\rangle = -(2\pi)^3 2\omega_{\mathbf{k}}\delta^{(3)}(0)\,. \tag{3.127}$$

Related to this is the fact that the $\lambda = 0$ contribution to the Hamiltonian:

$$H = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3 2\omega_{\mathbf{k}}} k^0 \left\{ \sum_{\lambda=1}^{3} a^{(\lambda)\dagger}(\mathbf{k})a^{(\lambda)}(\mathbf{k}) - a^{(0)\dagger}(\mathbf{k})a^{(0)}(\mathbf{k}) \right\}, \tag{3.128}$$

is negative. Fortunately, these problems are resolved when we take the Lorentz gauge (3.117) into account. However, it cannot be satisfied as an operator equation because it is inconsistent with the commutation relations. Instead, we could try imposing the weaker requirement that

$$\partial_\mu A^\mu|\psi\rangle = [\partial_\mu A^{(+)\mu} + \partial_\mu A^{(-)\mu}]|\psi\rangle = 0\,, \tag{3.129}$$

for all physical states $|\psi\rangle$. But this equation cannot be satisfied even for the vacuum state because the negative frequency operator $A^{(-)}$ contains creation operators, making it non-zero. So we impose the even less demanding requirement:

$$\partial_\mu A^{(+)\mu}|\psi\rangle = 0\,. \tag{3.130}$$

In particular, the vacuum automatically satisfies this since $A^{(+)}$ contains annihilation operators. It follows that the expectation value of $\partial_\mu A^\mu$ in any physical state $|\psi\rangle$ vanishes:

$$\begin{aligned}
\langle\psi|\partial_\mu A^\mu|\psi\rangle &= \langle\psi|\partial_\mu A^{(+)\mu} + \partial_\mu A^{(-)\mu}|\psi\rangle \\
&= \langle\psi|\partial_\mu A^{(-)\mu}|\psi\rangle \\
&= \langle\psi|\partial_\mu A^{(+)\mu}|\psi\rangle^* \\
&= 0\,.
\end{aligned} \tag{3.131}$$

To see how this resolves the problem of negative field density, we substitute the expansion for A^μ into (3.130) to get

$$\sum_{\lambda=0}^{3} k^\mu \varepsilon_\mu^{(\lambda)} a^{(\lambda)}(\mathbf{k})|\psi\rangle = 0\,, \tag{3.132}$$

i.e.,

$$[k^\mu \varepsilon_\mu^{(0)} a^{(0)}(\mathbf{k}) + k^\mu \varepsilon_\mu^{(3)} a^{(3)}(\mathbf{k})]|\psi\rangle = 0\,. \tag{3.133}$$

But $k^\mu \varepsilon_\mu^{(0)} = -k^\mu \varepsilon_\mu^{(3)}$ from (3.123), so

$$[a^{(0)}(\mathbf{k}) - a^{(3)}(\mathbf{k})]|\psi\rangle = 0\,. \tag{3.134}$$

It follows that

$$\langle\psi|a^{(0)\dagger}(\mathbf{k})a^{(0)}(\mathbf{k})|\psi\rangle = \langle\psi|a^{(3)\dagger}(\mathbf{k})a^{(3)}(\mathbf{k})|\psi\rangle\,, \tag{3.135}$$

i.e., the number of scalar photons is the same as the number of longitudinal ones. This means that the contributions of the scalar and longitudinal photons to the Hamiltonian (3.128) cancel each other, leaving only contributions of the transverse states, which are of course, positive-definite.

A physical state thus consists of transverse photons, with n scalar and n longitudinal photons. The subspace of states with different n all correspond to the same physics; so we can choose $n = 0$ without loss of generality.

We can recast this formalism in a gauge-invariant form, in terms of $F_{\mu\nu}$, by requiring

$$F_{\mu\nu}^{(+)}|\psi\rangle = 0\,, \tag{3.136}$$

instead of (3.130). In a frame such that $k^\mu = (k, 0, 0, k)$, this condition is equivalent to $k(a^{(0)} - a^{(3)})|\psi\rangle = 0$. The Lagrangian given by (3.112). This differs from the previous form by a divergence, which contributes a surface integral to the action and so does not affect the field equation.

3.7 References and further reading

I have based this chapter on the excellent treatments of Ryder, *Quantum Field Theory*, and Mandl and Shaw, with the same title. Another good reference is Peskin and Schroeder, *An Introduction to Quantum Field Theory*.