

## 2 Quantization of the scalar field

**Commutator relations.** The strategy to quantize a classical field theory is to interpret the fields  $\Phi(x)$  and  $\Pi(x) = \dot{\Phi}(x)$  as operators which satisfy canonical commutation relations. This is completely analogous to the transition from classical to quantum mechanics for discrete systems, where  $q_i$  and  $p_i$  are promoted to self-adjoint operators that satisfy

$$[q_i, p_j] = i\delta_{ij}, \quad [q_i, q_j] = [p_i, p_j] = 0. \quad (2.1)$$

These relations hold in the Schrödinger picture where the time dependence is carried by the states alone; in the Heisenberg picture the operators are time-dependent and the commutation relations are imposed at equal times. In the following we will always work in the Heisenberg picture, so we demand that for equal times

$$\begin{aligned} [\Phi(x), \Pi(y)]_{x^0=y^0} &= i\delta^{(3)}(\mathbf{x} - \mathbf{y}), \\ [\Phi(x), \Phi(y)]_{x^0=y^0} &= [\Pi(x), \Pi(y)]_{x^0=y^0} = 0. \end{aligned} \quad (2.2)$$

Despite appearances, this does not destroy Lorentz covariance because  $x$  and  $y$  are separated by a spacelike distance  $(x - y)^2 < 0$  which is preserved under a Lorentz transformation. By virtue of the Dirac delta function,  $\Phi(x)$  and  $\Pi(x)$  are now operator-valued distributions; to arrive at well-defined expressions one should in principle ‘smear’ them with smooth test functions.

The wave functions in quantum mechanics are also fields  $\Phi(x)$  that satisfy (relativistic or non-relativistic) wave equations, but there they are interpreted as single-particle wave functions in some Hilbert space by imposing an appropriate scalar product. (Unfortunately, already for relativistic Klein-Gordon particles the scalar product is not positive definite, so we lost the probability interpretation). In quantum field theory we impose instead an operator structure on  $\Phi(x)$ , which is why the procedure is often called ‘second quantization’. Since we really only quantize the field  $\Phi(x)$  once, the correct term should be ‘field quantization’.

**Fourier expansion.** We write the Fourier expansion for solutions of the free Klein-Gordon equation as

$$\Phi(x) = \frac{1}{(2\pi)^{3/2}} \int \frac{d^3p}{2E_p} \left( a(\mathbf{p}) e^{-ipx} + a^\dagger(\mathbf{p}) e^{ipx} \right) \Big|_{p^0=E_p}, \quad (2.3)$$

so the Fourier coefficients (from now on we abbreviate  $a(\mathbf{p}) \equiv a_p$ ) will inherit the operator structure. In the following we will often encounter the Lorentz-invariant integral measure  $\int d^3p/(2E_p)$  that is obtained by restricting the four-momentum integration to the positive-energy mass shell (which is a Lorentz-invariant condition):

$$\int d^4p \Theta(p^0) \delta(p^2 - m^2) = \int d^4p \Theta(p^0) \frac{\delta(p^0 - E_p) + \delta(p^0 + E_p)}{2E_p} = \int \frac{d^3p}{2E_p}. \quad (2.4)$$

Consequently, also the combination  $2E_p \delta^3(\mathbf{p} - \mathbf{p}')$  is Lorentz-invariant. Upon inserting the Fourier expansion into Eq. (2.2) we obtain the commutation relations for  $a_p, a_{p'}^\dagger$ :

$$[a_p, a_{p'}^\dagger] = 2E_p \delta^{(3)}(\mathbf{p} - \mathbf{p}'), \quad [a_p, a_{p'}] = [a_p^\dagger, a_{p'}^\dagger] = 0. \quad (2.5)$$

This can be shown in several ways. For example, let's write

$$\begin{aligned}\Phi(x) &= \frac{1}{(2\pi)^{3/2}} \int d^3p \left( \frac{a_p e^{-iE_p t} + a_{-p}^\dagger e^{iE_p t}}{2E_p} \right) e^{i\mathbf{p}\cdot\mathbf{x}}, \\ \Pi(x) = \dot{\phi}(x) &= \frac{1}{(2\pi)^{3/2}} \int d^3p \left( \frac{a_p e^{-iE_p t} - a_{-p}^\dagger e^{iE_p t}}{2i} \right) e^{i\mathbf{p}\cdot\mathbf{x}},\end{aligned}\tag{2.6}$$

and abbreviate the two brackets (the three-dimensional Fourier transforms) by

$$\tilde{\Phi}_p(t) = \frac{1}{2E_p} (a_p(t) + a_{-p}^\dagger(t)), \quad \tilde{\Pi}_p(t) = \frac{1}{2i} (a_p(t) - a_{-p}^\dagger(t)).\tag{2.7}$$

It follows that

$$\begin{aligned}\tilde{\Phi}_p^\dagger(t) &= \tilde{\Phi}_{-p}(t), & a_p(t) &= E_p \tilde{\Phi}_p(t) + i \tilde{\Pi}_p(t), \\ \tilde{\Pi}_p^\dagger(t) &= \tilde{\Pi}_{-p}(t), & a_p^\dagger(t) &= E_p \tilde{\Phi}_p^\dagger(t) - i \tilde{\Pi}_p^\dagger(t).\end{aligned}\tag{2.8}$$

Now insert this into the commutator:

$$[\Phi(x), \pi(y)]_{x^0=y^0} = \int \frac{d^3p d^3p'}{(2\pi)^3} e^{i(\mathbf{p}\cdot\mathbf{x} - \mathbf{p}'\cdot\mathbf{y})} [\tilde{\Phi}_p(t), \tilde{\Pi}_{p'}^\dagger(t)] \stackrel{!}{=} i\delta^{(3)}(\mathbf{x} - \mathbf{y}).\tag{2.9}$$

Here we have changed the integration variable from  $\mathbf{p} \rightarrow -\mathbf{p}$  and used  $\tilde{\Pi}_{-p}(t) = \tilde{\Pi}_p^\dagger(t)$ . Hence, the commutator for the Fourier transformed quantities must be also a  $\delta$ -function (the time dependence cancels),

$$[\tilde{\Phi}_p(t), \tilde{\Pi}_{p'}^\dagger(t)] = i\delta^{(3)}(\mathbf{p} - \mathbf{p}'),\tag{2.10}$$

and we can extract the commutator relation for  $a_p$  and  $a_{p'}^\dagger$ :

$$[a_p, a_{p'}^\dagger] = [a_p(t), a_{p'}^\dagger(t)] = -iE_p [\tilde{\Phi}_p(t), \tilde{\Pi}_{p'}^\dagger(t)] + iE_{p'} [\tilde{\Phi}_{p'}^\dagger(t), \tilde{\Pi}_p^\dagger(t)]^\dagger = 2E_p \delta^{(3)}(\mathbf{p} - \mathbf{p}').\tag{2.11}$$

Another way to arrive at this result is to use Eq. (1.27) for the Fourier coefficients and calculate the commutator directly:

$$a_p = \langle f_p, \Phi \rangle = i \int d^3x f_p^*(x) \overleftrightarrow{\partial}_0 \Phi(x) \Big|_{x^0=t}, \quad a_p^\dagger = -\langle f_p^\dagger, \Phi \rangle = -i \int d^3x f_p(x) \overleftrightarrow{\partial}_0 \Phi(x) \Big|_{x^0=t}.\tag{2.12}$$

For equal times  $x^0 = y^0 = t$  we can insert the commutator relations (2.2), so that

$$\begin{aligned}[a_p, a_{p'}^\dagger] &= \int d^3x \int d^3y f_p^*(x) f_{p'}(y) \overleftrightarrow{\partial}_{x^0} \overleftrightarrow{\partial}_{y^0} [\Phi(x), \Phi(y)] \doteq \\ &= \int d^3x \int d^3y \left[ f_p^*(x) \dot{f}_{p'}(y) - \dot{f}_p^*(x) f_{p'}(y) \right] i\delta^3(\mathbf{x} - \mathbf{y}) \\ &= i \int d^3x f_p^*(x) \overleftrightarrow{\partial}_0 f_{p'}(x) = \langle f_p, f_{p'} \rangle = 2E_p \delta^3(\mathbf{p} - \mathbf{q}).\end{aligned}\tag{2.13}$$

**Hamilton and momentum operator.** To proceed, we derive the Fourier decomposition for the Hamiltonian (1.15) of the free scalar field theory. The form of the Hamiltonian already resembles that of a collection of harmonic oscillators at each point  $\mathbf{x}$ , but the term  $(\nabla\Phi)^2$  couples the degrees of freedom at  $\mathbf{x}$  and  $\mathbf{x} + \delta\mathbf{x}$ . We can diagonalize it in momentum space by inserting the relations (2.6–2.7); in that way it becomes the sum of decoupled harmonic oscillators with frequencies  $E_p$ :

$$H = \int d^3x \frac{1}{2} [\Pi^2 + (\nabla\Phi)^2 + m^2\Phi^2] = \int d^3p \frac{1}{2} \left[ \tilde{\Pi}_p^\dagger(t) \tilde{\Pi}_p(t) + E_p^2 \tilde{\Phi}_p^\dagger(t) \tilde{\Phi}_p(t) \right].\tag{2.14}$$

To arrive at this result, use

$$\begin{aligned}\int d^3x (\nabla\Phi)^2 &= \int d^3x \int \frac{d^3p d^3p'}{(2\pi)^3} \tilde{\Phi}_p(t) \tilde{\Phi}_{p'}(t) (-\mathbf{p} \cdot \mathbf{p}') e^{i(\mathbf{p}+\mathbf{p}')\cdot\mathbf{x}} \\ &= \int d^3p \tilde{\Phi}_p(t) \tilde{\Phi}_{-p}(t) \mathbf{p}^2 = \int d^3p \tilde{\Phi}_p^\dagger(t) \tilde{\Phi}_p(t) \mathbf{p}^2\end{aligned}\tag{2.15}$$

and similarly

$$\int d^3x \Phi^2 = \int d^3p \tilde{\Phi}_p^\dagger(t) \tilde{\Phi}_p(t), \quad \int d^3x \Pi^2 = \int d^3p \tilde{\Pi}_p^\dagger(t) \tilde{\Pi}_p(t). \quad (2.16)$$

Inserting the decomposition (2.7) finally yields the result

$$H = \int \frac{d^3p}{2E_p} E_p \frac{a_p^\dagger a_p + a_p a_p^\dagger}{2}. \quad (2.17)$$

Unfortunately this expression is divergent because it contains the sum of the zero-point energy of all oscillators:

$$\frac{a_p^\dagger a_p + a_p a_p^\dagger}{2} = a_p^\dagger a_p + \frac{1}{2} [a_p, a_p^\dagger] = a_p^\dagger a_p + E_p \delta^3(\mathbf{0}). \quad (2.18)$$

The Dirac delta is proportional to the volume; had we studied the system in a finite box, we would write  $(2\pi)^3 \delta^3(\mathbf{0}) \rightarrow V$ . (This is an **infrared divergence**.) However, for large  $\mathbf{p}$  we have  $E_p \sim \sqrt{\mathbf{p}^2 + m^2} \simeq |\mathbf{p}|$  and the integral still diverges. If we regulate the divergence by integrating only up to a cutoff  $|\mathbf{p}| \leq \Lambda$ , the energy density of the vacuum becomes

$$\rho_{\text{vac}} = \frac{E_{\text{vac}}}{V} = \frac{1}{2} \int \frac{d^3p}{(2\pi)^3} E_p \sim \int dp p^3 \sim \Lambda^4. \quad (2.19)$$

This is a first example of an **ultraviolet divergence** which we will frequently encounter later. Since (in a theory without gravity) we can only measure energy differences, we can simply discard it so that the vacuum energy is zero. This is formally called *normal ordering* or *Wick ordering*: we obtain the normal-ordered form  $:\mathcal{O}:$  of some operator  $\mathcal{O}$  by moving all creation operators to the left of all destruction operators. Later when we discuss renormalization we will see how UV divergences can be systematically removed from the theory; for the time being we interpret all operators as being normal-ordered. Hence, the Hamilton operator becomes

$$H = \int d^3x \frac{1}{2} :[\Pi^2 + (\nabla\Phi)^2 + m^2\Phi^2]: = \int \frac{d^3p}{2E_p} E_p a_p^\dagger a_p. \quad (2.20)$$

We can repeat the procedure to obtain the spatial momentum operator  $\mathbf{P}$ . We identify it with the classical charge  $P^i = \int d^3x T^{0i}$  in Eq. (1.50) that follows from the invariance under spatial translations. The analogous calculation gives

$$\mathbf{P} = - \int d^3x : \Pi \nabla \Phi : = i \int d^3p \mathbf{p} : \tilde{\Pi}_p(t) \tilde{\Phi}_p^\dagger(t) : = \int \frac{d^3p}{2E_p} \mathbf{p} a_p^\dagger a_p, \quad (2.21)$$

so that we can combine Eqs. (2.20) and (2.21) into the covariant four-momentum operator

$$P^\mu = \int d^3x : T^{0\mu} : = \int \frac{d^3p}{2E_p} p^\mu a_p^\dagger a_p \Big|_{p^0=E_p}. \quad (2.22)$$

**Fock space.** What is the Hilbert space on which the four-momentum operator acts? Since  $P^\mu$  is self-adjoint it has eigenstates with real eigenvalues. Let  $|k\rangle$  be such an eigenstate with  $P^\mu |k\rangle = k^\mu |k\rangle$ , so that  $\mathbf{k}$  is the momentum of the state and  $k^0 = E_k$  its energy. First we observe that the energy (and therefore  $H$  itself) is non-negative:

$$\langle \lambda | H | \lambda \rangle = \int \frac{d^3 p}{2E_p} E_p \langle \lambda | a_p^\dagger a_p | \lambda \rangle \geq 0, \quad (2.23)$$

because the integrand is  $||a_p | \lambda \rangle||^2$ . On the other hand, we can calculate the commutators

$$[P^\mu, a_q^\dagger] = q^\mu a_q^\dagger, \quad [P^\mu, a_q] = -q^\mu a_q \quad (2.24)$$

and use them to show that if  $|k\rangle$  is an eigenstate of  $P^\mu$ , then also  $a_q^\dagger |k\rangle$  and  $a_q |k\rangle$  are eigenstates of  $P^\mu$  with their eigenvalues shifted by the momentum  $\pm q^\mu$ :

$$\begin{aligned} P^\mu (a_q^\dagger |k\rangle) &= a_q^\dagger (P^\mu + q^\mu) |k\rangle = (k + q)^\mu a_q^\dagger |k\rangle, \\ P^\mu (a_q |k\rangle) &= a_q (P^\mu - q^\mu) |k\rangle = (k - q)^\mu a_q |k\rangle, \end{aligned} \quad (2.25)$$

which at the same time shifts the energy of the state. Hence we can interpret  $a_q^\dagger, a_q$  as ladder operators. Since the total energy cannot be smaller than zero, there must be a state with  $a_q |0\rangle = 0 \forall \mathbf{q}$ , because otherwise the successive action of  $a_q$  would lead to negative eigenvalues of  $H$ .

We call  $|0\rangle$  the vacuum of the theory. It has four-momentum zero:  $P^\mu |0\rangle = 0$ , and we normalize it to  $\langle 0|0\rangle = 1$ . The state  $a_k^\dagger |0\rangle$  then has four-momentum  $k^\mu = (E_k, \mathbf{k})$ :

$$P^\mu a_k^\dagger |0\rangle = k^\mu a_k^\dagger |0\rangle. \quad (2.26)$$

Since  $E_k = \sqrt{\mathbf{k}^2 + m^2}$  is the relativistic dispersion relation for a single particle with mass  $m$ , we interpret  $|k\rangle = a_k^\dagger |0\rangle$  as a one-particle state with energy  $E_k$  and momentum  $\mathbf{k}$ . Its normalization is

$$\langle k | k' \rangle = \langle 0 | a_k a_{k'}^\dagger | 0 \rangle = \langle 0 | a_{k'}^\dagger a_k + 2E_k \delta^3(\mathbf{k} - \mathbf{k}') | 0 \rangle = 2E_k \delta^3(\mathbf{k} - \mathbf{k}') \quad (2.27)$$

which, in turn, leads to the Lorentz-invariant completeness relation on the one-particle Hilbert space:

$$\mathbb{1}_{\text{1-particle}} = \int \frac{d^3 k}{2E_k} |k\rangle \langle k|. \quad (2.28)$$

Similarly, for a two-particle state we obtain

$$P^\mu a_q^\dagger a_k^\dagger |0\rangle = (q^\mu + k^\mu) a_q^\dagger a_k^\dagger |0\rangle \quad (2.29)$$

and so on. A generic  $N$ -particle state has the form  $|k_1 \dots k_N\rangle = a_{k_1}^\dagger \dots a_{k_N}^\dagger |0\rangle$ , and the eigenvalue of the momentum operator is the total momentum of the system:

$$P^\mu |k_1 \dots k_N\rangle = (k_1^\mu + \dots + k_N^\mu) |k_1 \dots k_N\rangle. \quad (2.30)$$

The resulting *Fock space* is the direct sum of all  $N$ -particle Hilbert spaces ( $N \in \mathbb{N}_0$ ). From the fact that the creation operators commute between themselves we also see that

these multiparticle states are symmetric under the exchange of any two particles, so they obey Bose–Einstein statistics. This is an example of the spin-statistics theorem, which states that particles with integer spin are bosons and particles with half-integer spin are fermions.

Generally, a multiparticle state that contains  $K$  different momenta  $k_i$ ,  $i = 1 \dots K$ , with  $n(k_i)$  particles carrying momentum  $k_i$  and  $\sum_{i=1}^K n(k_i)$  particles in total, can be written as

$$|n(k_1) n(k_2) \dots n(k_K)\rangle = \prod_{i=1}^K \frac{(a_{k_i}^\dagger)^{n(k_i)}}{\sqrt{n(k_i)!}} |0\rangle, \quad (2.31)$$

where the denominator takes care of multiplicities in the same momentum. We can count the total number of particles in such a state with the number operator

$$N = \int \frac{d^3p}{2E_p} a_p^\dagger a_p. \quad (2.32)$$

The eigenvalues of the operators  $N$  and  $P^\mu$  are the total number of particles and the total four-momentum, respectively:

$$N \rightarrow \sum_{i=1}^K n(k_i), \quad P^\mu \rightarrow \sum_{i=1}^K n(k_i) k_i^\mu. \quad (2.33)$$

This can be easily proven for  $K = 1$ , i.e., for a state  $|n(k)\rangle$  that consists of  $n(k)$  identical particles with momentum  $k$ : simply commute  $a_p$  in Eqs. (2.22) and (2.32) to the right until it annihilates on the vacuum. The eigenvalue of  $N$  is  $n(k)$  and the total momentum is  $n(k) k^\mu$ , and therefore the total energy  $n(k)E_k$  is the sum of the energies of all particles.

We can now also better understand the meaning of the field  $\Phi(x)$ . Written in Fourier modes (2.3) and acting on the vacuum, it creates a particle at the position  $x$ :

$$\Phi(x)|0\rangle = \frac{1}{(2\pi)^{3/2}} \int \frac{d^3p}{2E_p} e^{ipx} |p\rangle \Big|_{p^0=E_p} = |x\rangle, \quad (2.34)$$

and with the normalization (2.27) we can write the one-particle ‘wave function’ as the overlap

$$\langle x|p\rangle = \langle 0|\Phi(x)|p\rangle = \frac{1}{(2\pi)^{3/2}} e^{-ipx} \Big|_{p^0=E_p}. \quad (2.35)$$

In that way the fundamental entities in quantum field theory are not the particles but rather the field  $\Phi(x)$  which penetrates spacetime. Although it is not measurable by itself, we can interpret it as the ‘property of spacetime’ to create particles of momentum  $\mathbf{p}$  and energy  $E_p$  as its excitations.

**Complex scalar field and antiparticles.** Let’s generalize the formalism to complex scalar fields  $\Phi(x)$  and  $\Phi^\dagger(x)$ , because this will allow us to describe not only particles but also their antiparticles. The Lagrangian has the form

$$\mathcal{L} = \partial_\mu \Phi^\dagger \partial^\mu \Phi - m^2 \Phi^\dagger \Phi, \quad (2.36)$$

the conjugate momenta become

$$\Pi(x) = \frac{\partial \mathcal{L}}{\partial \dot{\Phi}(x)} = \dot{\Phi}^\dagger(x), \quad \Pi^\dagger(x) = \frac{\partial \mathcal{L}}{\partial \dot{\Phi}^\dagger(x)} = \dot{\Phi}(x) \quad (2.37)$$

and the Hamiltonian is

$$H = \int d^3x \left( \Pi^\dagger \dot{\Phi}^\dagger + \Pi \dot{\Phi} - \mathcal{L} \right) = \int d^3x \left( \Pi^\dagger \Pi + \nabla \Phi^\dagger \nabla \Phi + m^2 \Phi^\dagger \Phi \right). \quad (2.38)$$

The commutator relations are

$$\left[ \Phi(x), \Pi(y) \right]_{x^0=y^0} = \left[ \Phi^\dagger(x), \Pi^\dagger(y) \right]_{x^0=y^0} = i\delta^3(\mathbf{x} - \mathbf{y}) \quad (2.39)$$

whereas all other commutators vanish. The Fourier expansion has now the form

$$\begin{aligned} \Phi(x) &= \frac{1}{(2\pi)^{3/2}} \int \frac{d^3p}{2E_p} \left( a_p e^{-ipx} + b_p^\dagger e^{ipx} \right) \Big|_{p^0=E_p}, \\ \Phi^\dagger(x) &= \frac{1}{(2\pi)^{3/2}} \int \frac{d^3p}{2E_p} \left( b_p e^{-ipx} + a_p^\dagger e^{ipx} \right) \Big|_{p^0=E_p} \end{aligned} \quad (2.40)$$

with independent operators  $a_p$  and  $b_p$  whose commutation relations become

$$[a_p, a_{p'}^\dagger] = [b_p, b_{p'}^\dagger] = 2E_p \delta^3(\mathbf{p} - \mathbf{p}'), \quad (2.41)$$

with all others zero. The mode expansion of the four-momentum operator is

$$P^\mu = \int \frac{d^3p}{2E_p} p^\mu \left( a_p^\dagger a_p + b_p^\dagger b_p \right) \quad (2.42)$$

and implies that there are now two types of particles, with two types of momentum eigenstates  $a_p^\dagger |0\rangle$  and  $b_p^\dagger |0\rangle$  which have the same momentum  $\mathbf{p}$ , energy  $E_p = \sqrt{\mathbf{p}^2 + m^2}$  and mass  $m$ . Since they are scalar particles they also have both spin zero. So what distinguishes them?

There is a new property that is particular to the Lagrangian for a complex scalar field: is invariant under the continuous global  $U(1)$  symmetry

$$\Phi'(x) = e^{i\varepsilon} \Phi(x), \quad \Phi'^\dagger(x) = e^{-i\varepsilon} \Phi^\dagger(x), \quad (2.43)$$

with  $\varepsilon \in \mathbb{R}$  constant. According to Noether's theorem there is now a conserved current

$$j^\mu = i : (\Phi^\dagger \partial^\mu \Phi - \partial^\mu \Phi^\dagger \Phi) : \quad (2.44)$$

whose corresponding charge is

$$Q = \int d^3x j^0 = i \int d^3x : (\Phi^\dagger \dot{\Phi} - \dot{\Phi}^\dagger \Phi) : = \int \frac{d^3p}{2E_p} \left( a_p^\dagger a_p - b_p^\dagger b_p \right). \quad (2.45)$$

Comparing this with Eq. (2.32), we see that the  $U(1)$  charge describes the total number of particles created by  $a_p^\dagger$  minus that created by  $b_p^\dagger$ , which is conserved. For example, its eigenvalues for one-particle states are

$$Q a_p^\dagger |0\rangle = a_p^\dagger |0\rangle, \quad Q b_p^\dagger |0\rangle = -b_p^\dagger |0\rangle. \quad (2.46)$$

We will call them particles and antiparticles; for the real field the particle is its own antiparticle. Now we can also interpret the negative-energy solutions of the Klein-Gordon equation: via Eq. (2.40) the coefficient of the positive-energy solution  $e^{-ipx}$

becomes the annihilation operator of a particle and that of  $e^{ipx}$  the creation operator of its antiparticle. In the context of QED we will later find that the  $U(1)$  Noether charge indeed corresponds to the *electric* charge, i.e., the coupling to the electromagnetic field.

**Poincaré algebra.** In our discussion of the Poincaré group we saw that Poincaré transformations have the form

$$x' = T(\Lambda, a)x = \Lambda x + a \quad \Leftrightarrow \quad \delta x^\mu = \varepsilon^{\mu\nu} x_\nu + a^\mu. \quad (2.47)$$

The group axioms are satisfied: the transformation is associative,  $(TT')T'' = T(T'T'')$ , the unit element is  $T(1, 0)$ , two consecutive Poincaré transformations form another one:  $T(\Lambda', a')T(\Lambda, a) = T(\Lambda'\Lambda, a' + \Lambda'a)$ , and from equating this with  $T(1, 0)$  we can read off the inverse element:  $T^{-1}(\Lambda, a) = T(\Lambda^{-1}, -\Lambda^{-1}a)$ .

Consider now the representations  $U(\Lambda, a)$  of the Poincaré group on some vector space. They inherit the group structure from the  $T(\Lambda, a)$ , and we use the symbol  $U$  although they are not necessarily unitary. The Poincaré group  $ISO(3, 1)^\uparrow$  is a Lie group and therefore its elements can be written as

$$U(\Lambda, a) = e^{\frac{i}{2}\varepsilon_{\mu\nu} M^{\mu\nu}} e^{ia_\mu P^\mu} = 1 + \frac{i}{2}\varepsilon_{\mu\nu} M^{\mu\nu} + ia_\mu P^\mu + \dots, \quad (2.48)$$

with infinitesimal generators  $M^{\mu\nu}$  for Lorentz transformations and  $P^\mu$  for translations. Their explicit form depends on the representation, i.e., it is determined by the vector space on which they act. Since  $\varepsilon_{\mu\nu}$  is totally antisymmetric,  $M^{\mu\nu}$  can also be chosen antisymmetric. It contains the six generators of the Lorentz group, whereas the momentum operator  $P^\mu$  is the generator of spacetime translations.  $M^{\mu\nu}$  and  $P^\mu$  form a Lie algebra (the Poincaré algebra) whose commutator relations are given by

$$i[M^{\mu\nu}, M^{\rho\sigma}] = g^{\mu\sigma} M^{\nu\rho} + g^{\nu\rho} M^{\mu\sigma} - g^{\mu\rho} M^{\nu\sigma} - g^{\nu\sigma} M^{\mu\rho}, \quad (2.49)$$

$$i[P^\mu, M^{\rho\sigma}] = g^{\mu\rho} P^\sigma - g^{\mu\sigma} P^\rho, \quad (2.50)$$

$$[P^\mu, P^\nu] = 0. \quad (2.51)$$

These relations can be derived from

**(Ex)**

$$U(\Lambda, a)U(\Lambda', a')U^{-1}(\Lambda, a) = U(\Lambda\Lambda'\Lambda^{-1}, a + \Lambda a' - \Lambda\Lambda'\Lambda^{-1}a), \quad (2.52)$$

which follows from the composition rules for the  $T(\Lambda, a)$ : insert infinitesimal transformations (2.48) for each  $U(\Lambda = 1 + \varepsilon, a)$ , with  $U^{-1}(\Lambda, a) = U(1 - \varepsilon, -a)$ , keep only linear terms in all group parameters  $\varepsilon, \varepsilon', a$  and  $a'$ , and compare coefficients of the terms  $\sim \varepsilon\varepsilon', a\varepsilon', \varepsilon a'$  and  $aa'$ . A shortcut to arrive at the Lorentz algebra relation (2.49) is to calculate the generator  $M^{\mu\nu}$  directly in the four-dimensional representation, where  $U(\Lambda, 0) = \Lambda$  is the Lorentz transformation itself:

$$U(\Lambda, 0)^\alpha_\beta = \delta^\alpha_\beta + \frac{i}{2}\varepsilon_{\mu\nu} (M^{\mu\nu})^\alpha_\beta + \dots = \Lambda^\alpha_\beta = \delta^\alpha_\beta + \varepsilon^\alpha_\beta + \dots \quad (2.53)$$

This is solved by the tensor

$$(M^{\mu\nu})^\alpha_\beta = -i(g^{\mu\alpha}\delta^\nu_\beta - g^{\nu\alpha}\delta^\mu_\beta) \quad (2.54)$$

which satisfies the commutator relation (2.49).

We can cast the Poincaré algebra relations in a less compact but more useful form. The antisymmetric matrix  $\varepsilon_{\mu\nu}$  contains the six group parameters and the antisymmetric matrix  $M^{\mu\nu}$  the six generators. If we define the generator of  $SO(3)$  rotations  $\mathbf{J}$  (the angular momentum) and the generator of boosts  $\mathbf{K}$  via

$$M^{ij} = -\varepsilon_{ijk} J^k \quad \Leftrightarrow \quad J^i = -\frac{1}{2}\varepsilon_{ijk} M^{jk}, \quad M^{0i} = K^i, \quad (2.55)$$

then the commutator relations take the form

$$\begin{aligned}
[J^i, J^j] &= i\varepsilon_{ijk} J^k, & [J^i, P^j] &= i\varepsilon_{ijk} P^k, & [P^i, P^j] &= 0, \\
[J^i, K^j] &= i\varepsilon_{ijk} K^k, & [K^i, P^j] &= i\delta_{ij} P_0, & [J^i, P_0] &= 0, \\
[K^i, K^j] &= -i\varepsilon_{ijk} J^k, & [K^i, P_0] &= iP^i, & [P^i, P_0] &= 0.
\end{aligned}
\tag{2.56}$$

Here we see that boosts and rotations generally do not commute unless the boost and rotation axes coincide. Moreover,  $P_0$  (which is the Hamilton operator in the quantum field theory) commutes with rotations and spatial translations but not with boosts and therefore the eigenvalues of  $\mathbf{K}$  cannot be used for labeling physical states. If we similarly define  $\varepsilon_{ij} = -\varepsilon_{ijk} \phi^k$  and  $\varepsilon_{0i} = s^i$ , we obtain

$$\frac{i}{2} \varepsilon_{\mu\nu} M^{\mu\nu} = i\boldsymbol{\phi} \cdot \mathbf{J} + i\mathbf{s} \cdot \mathbf{K} . \tag{2.57}$$

$\mathbf{J}$  is hermitian but  $\mathbf{K}$  is antihermitian for all finite-dimensional representations, which prevents them from being unitary: there are no finite-dimensional unitary representations of the Lorentz and Poincaré groups. This is a consequence of the fact that the Lorentz group is not compact: it contains the boosts whose parameter space is isomorphic to  $\mathbb{R}^3$ . Later will discuss explicit examples for  $\mathbf{K}$  when considering spinor representations.

**Representation on the Fock space.** How is the Poincaré group represented on the Fock space? It is not an accident that we chose the same symbol  $P^\mu$  for the generator of translations *and* for the classical Noether charge in Eq. (1.51), which meanwhile has also become the momentum operator in the quantum field theory. It turns out that, after quantizing the theory, the classical constants of motion  $P^\mu$  and  $M^{\mu\nu}$  become self-adjoint operators on the Fock space which define a unitary representation of the Poincaré group.<sup>2</sup> This means they satisfy the same Poincaré algebra relations as in Eqs. (2.49–2.51), which happens to be a consequence of the commutation relations for the fields, and the corresponding operator  $U(\Lambda, a)$  is unitary.

In Eqs. (1.31–1.32) we have seen how classical fields behave under Poincaré transformations. The general transformation behavior of a collection of field *operators*  $\Phi_i(x)$  under Poincaré transformations is imposed as an *axiom* of quantum field theory:

$$U(\Lambda, a) \Phi_i(x) U(\Lambda, a)^{-1} = D(\Lambda)_{ij}^{-1} \Phi_j(\Lambda x + a) . \tag{2.58}$$

It ensures that matrix elements of field operators transform as

$$\langle \lambda'_1 | \Phi_i(x') | \lambda'_2 \rangle = \langle \lambda_1 | U(\Lambda, a)^{-1} \Phi_i(x') U(\Lambda, a) | \lambda_2 \rangle \stackrel{!}{=} D(\Lambda)_{ij} \langle \lambda_1 | \Phi_j(x) | \lambda_2 \rangle . \tag{2.59}$$

This can be generalized to products of field operators at different spacetime points, which gives the transformation behavior of correlation functions. We will discuss the consequences of Eq. (2.58) in more detail later in the context of the Dirac field. For the moment we restrict ourselves to a single scalar field where the equation reduces to

$$U(\Lambda, a) \Phi(x) U(\Lambda, a)^{-1} = \Phi(\Lambda x + a) . \tag{2.60}$$

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<sup>2</sup>Unitarity of  $U(\Lambda, a)$  has now become possible because the Fock space is infinite-dimensional.



In particular, for translations  $U(1, a) = e^{ia_\mu P^\mu}$  it takes the form

$$e^{ia_\mu P^\mu} \Phi(x) e^{-ia_\mu P^\mu} = \Phi(x + a). \quad (2.61)$$

Expanding both sides of the equation to  $\mathcal{O}(a)$  we obtain

$$\Phi(x) + ia_\mu [P^\mu, \Phi(x)] + \dots = \Phi(x) + a_\mu \partial^\mu \Phi(x) + \dots \quad (2.62)$$

from where we obtain the **Heisenberg equations of motion**:

$$\partial_\mu \Phi(x) = i[P_\mu, \Phi(x)]. \quad (2.63)$$

Since they follow from translation invariance they are quite general: they do not only hold for scalar fields but also for polynomials in  $\Phi$ , and more generally also for the individual components of fields with higher spin because each component behaves like a scalar field under translations. In particular, we can read off the Heisenberg equation for the time evolution which is known from quantum mechanics:

$$\frac{\partial \Phi(x)}{\partial t} = i[H, \Phi(x)]. \quad (2.64)$$

From the Heisenberg equations for  $\Phi(x)$  and  $\Pi(x)$  one can further recover the Klein-Gordon equation for the field  $\Phi(x)$ .

The analogue of Eq. (2.61) derived from Lorentz invariance has the form

$$e^{\frac{i}{2}\varepsilon_{\mu\nu} M^{\mu\nu}} \Phi(x) e^{-\frac{i}{2}\varepsilon_{\mu\nu} M^{\mu\nu}} = \Phi(\Lambda x), \quad (2.65)$$

with  $\Lambda = 1 + \varepsilon + \dots$ . Expanding both sides to  $\mathcal{O}(\varepsilon)$  and exploiting the antisymmetry of  $\varepsilon_{\mu\nu}$  yields the equation

$$i(x_\mu \partial_\nu - x_\nu \partial_\mu) \Phi(x) = [M_{\mu\nu}, \Phi(x)]. \quad (2.66)$$

**Causality.** The basic postulate of quantum field theory is that two measurements at spacelike distances should not affect each other. This is guaranteed if any two local observables  $\mathcal{O}_1(x)$  and  $\mathcal{O}_2(y)$  at spacelike separation commute, i.e.,

$$[\mathcal{O}_1(x), \mathcal{O}_2(y)] \stackrel{!}{=} 0 \quad \text{if } (x - y)^2 < 0. \quad (2.67)$$

To this end, consider the commutator of two fields at arbitrary times:

$$\Delta(x - y) := [\Phi(x), \Phi(y)]. \quad (2.68)$$

This quantity is known by various names: Pauli-Jordan function, Schwinger's  $\Delta$  function, or simply causal propagator. If we insert the Fourier decomposition (2.3) for free fields, use the commutator relation (2.5) and set  $z = x - y$ , we immediately get

$$\Delta(z) = \frac{1}{(2\pi)^3} \int \frac{d^3 p}{2E_p} (e^{-ipz} - e^{ipz}) \Big|_{p^0=E_p}. \quad (2.69)$$

Now observe this: for  $z^0 = 0$ ,  $\Delta(z)$  vanishes because in that case we can change the integration variable from  $\mathbf{p} \rightarrow -\mathbf{p}$  and the difference cancels. On the other hand,  $\Delta(z)$  is Lorentz-invariant because both  $e^{\pm i\mathbf{p}z}$  and the integral measure  $d^3p/(2E_p)$  are Lorentz-invariant. A Lorentz-invariant quantity that vanishes for  $z^0 = 0$  must vanish for all spacelike  $z$  with  $z^2 < 0$ , because they can all be reached by a Lorentz transformation. Hence,  $\Delta(z)$  has only support inside the light cone ( $z^2 \geq 0$ ).

In an interacting quantum field theory we cannot use a free mode expansion anymore to calculate  $\Delta(z)$ . In that case we also have to postulate **microcausality** as an axiom:

$$[\Phi(x), \Phi(y)] = 0 \quad \text{if } (x - y)^2 < 0. \quad (2.70)$$

This also generalizes our earlier commutation relations (2.2) because they can be derived from it:  $\partial_0 \Delta(z)|_{z^0=0} = -i\delta^3(\mathbf{z})$ . Of course  $\Phi(x)$  is not a measurable quantity but actual observables like currents, charges etc. are functions of the fields and therefore inherit its causal properties.

**Propagators.** Consider now the quantity

$$D(x - y) := \langle 0 | \Phi(x) \Phi(y) | 0 \rangle. \quad (2.71)$$

Since  $\Phi(x) | 0 \rangle = | x \rangle$ , this is the amplitude  $\langle x | y \rangle$  for a particle that is emitted at  $y$  and propagates to  $x$ . Its analogue in nonrelativistic quantum mechanics is the amplitude  $\langle \mathbf{x} | e^{-iHt} | \mathbf{y} \rangle$ , which is nonzero even if  $x - y$  is spacelike (hence the problem with causality in quantum mechanics).<sup>3</sup> If we insert the Fourier decomposition (2.3) into  $D(x - y)$  then, because we act on the vacuum on both sides, the only term that survives is  $\langle 0 | a_p a_p^\dagger | 0 \rangle = \langle p | p' \rangle = 2E_p \delta^3(\mathbf{p} - \mathbf{p}')$  and we arrive at

$$D(z) = \frac{1}{(2\pi)^3} \int \frac{d^3p}{2E_p} e^{-ipz} \Big|_{p^0=E_p}. \quad (2.72)$$

This expression is again Lorentz-invariant but nonzero for  $z^0 = 0$ , so it is generally also nonzero for spacelike distances  $z^2 < 0$ . How is this compatible with causality? The crucial observation is that the commutator

$$[\Phi(x), \Phi(y)] = D(x - y) - D(y - x) \quad (2.73)$$

describes two physical processes (propagation from  $y \rightarrow x$  and  $x \rightarrow y$ ) whose amplitudes cancel each other for  $(x - y)^2 < 0$ . This makes indeed sense because both processes can occur: if  $x - y$  is spacelike, there is no Lorentz-invariant notion of whether  $x^0 - y^0$  is larger or smaller than zero.

We can understand this better if we consider a *complex* scalar field where the Fourier decomposition of the field  $\Phi(x)$  contains  $a_p$ ,  $b_p^\dagger$  and  $\Phi^\dagger(x) \sim b_p$ ,  $a_p^\dagger$ . In that case we have to modify the axiom (2.70) so that it becomes

$$\Delta(x - y) = [\Phi(x), \Phi^\dagger(y)] = 0 \quad \text{if } (x - y)^2 < 0, \quad (2.74)$$

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<sup>3</sup>We do not need to insert the time-evolution operator in  $D(x - y)$  because  $|x\rangle$  already contains information about the time variable  $x^0$ .

whereas  $[\Phi(x), \Phi(y)] = 0 \forall x, y$ . The result for  $\Delta(z)$  in Eq. (2.69) remains the same, but now we have

$$[\Phi(x), \Phi^\dagger(y)] = \langle 0 | \Phi(x) \Phi^\dagger(y) | 0 \rangle - \langle 0 | \Phi^\dagger(y) \Phi(x) | 0 \rangle. \quad (2.75)$$

The first term corresponds to a particle that travels from  $y \rightarrow x$  and the second term to an *antiparticle* travelling from  $x \rightarrow y$ , and both processes cancel each other in the commutator. Therefore, it is really the multiparticle nature of quantum field theory that saves causality: the particle and antiparticle propagation cancel each other. (For a real scalar field  $\Phi(x) = \Phi^\dagger(x)$  the particle is its own antiparticle.)

**Feynman propagator.** Taking this idea further, we define the Feynman propagator

$$D_F(x - y) := \langle 0 | \mathbb{T} \Phi(x) \Phi^\dagger(y) | 0 \rangle = \begin{cases} \langle 0 | \Phi(x) \Phi^\dagger(y) | 0 \rangle & \text{if } x^0 \geq y^0, \\ \langle 0 | \Phi^\dagger(y) \Phi(x) | 0 \rangle & \text{if } y^0 \geq x^0, \end{cases} \quad (2.76)$$

where the time-ordering  $\mathbb{T}$  of some product of field operators implies that they should be ordered with increasing times from right to left. The Feynman propagator will become extremely important later because it is the fundamental quantity that appears in the Feynman rules for  $S$ -matrix elements. It describes the propagation of a particle forward in time, but simultaneously also the propagation of an antiparticle ‘backward in time’; hence, these two processes are physically the same.

The various propagators that we encountered are also called **Green’s functions** because they are the Green functions of the Klein-Gordon equation:

$$(\square + m^2) iD(z) = \delta^4(z). \quad (2.77)$$

We can find the general solution to this equation by taking the Fourier transform of both sides:

$$D(z) = \frac{1}{(2\pi)^4} \int d^4p \tilde{D}(p) e^{-ipz}, \quad \delta^4(z) = \frac{1}{(2\pi)^4} \int d^4p e^{-ipz}, \quad (2.78)$$

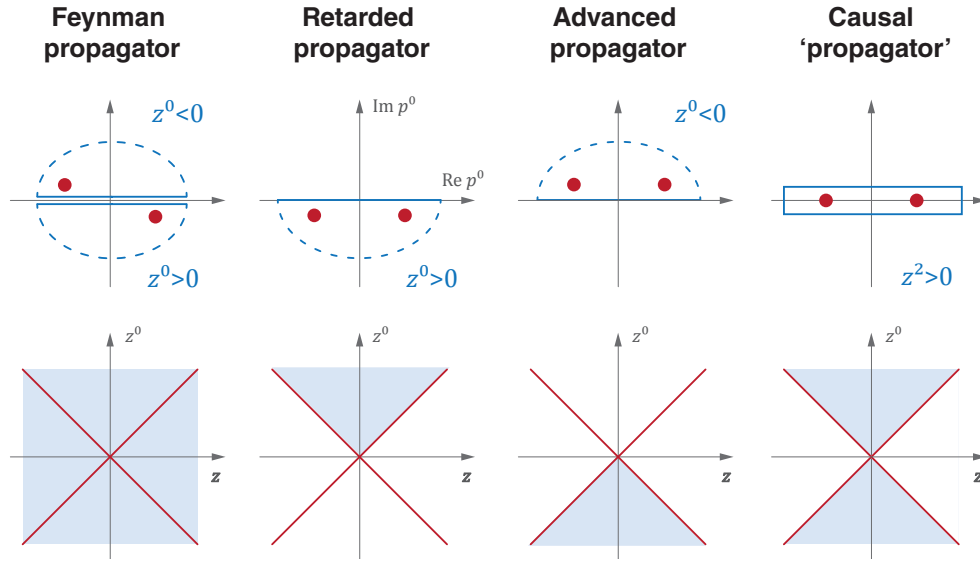
so that the propagator in momentum space becomes

$$\tilde{D}(p) = \frac{i}{p^2 - m^2}. \quad (2.79)$$

It has a pole on the real axis of  $p^2 = m^2$  or, equivalently, two poles at positive and negative energies  $p^0 = \pm E_p = \pm \sqrt{\mathbf{p}^2 + m^2}$ . The strategy in order to return the propagator to real space is to carry out the  $p^0$  integration first:

$$D(z) = i \int \frac{d^3p}{(2\pi)^4} e^{i\mathbf{p}\cdot\mathbf{z}} \int dp_0 \frac{e^{-ip_0 z_0}}{p_0^2 - E_p^2}. \quad (2.80)$$

The integral can be calculated by extending the real-axis integration to a closed contour in the complex  $p_0$  plane, which is allowed as long as the integrand vanishes at complex infinity. For  $z^0 > 0$  this holds as long as we close the contour in the lower half plane, whereas for  $z^0 < 0$  the integrand at infinity only vanishes if we close it in the upper half plane. Any consistent prescription to avoid divergences in performing this contour



**FIGURE 2.1:** Various integration contours in the complex  $p^0$  plane (top row) and support of the resulting propagators in the Minkowski diagram  $(z^0, |z|)$  (bottom row).

integral (there are  $2 \times 2$  different ways of doing so) leads to a solution of the original equation (2.77). By the residue theorem

$$\oint dz f(z) = 2\pi i \sum_n R(z_n), \quad R(z_0) = \lim_{z \rightarrow z_0} (z - z_0) f(z) \quad (2.81)$$

the result is  $(2\pi i)$  times the sum of the residues at  $p^0 = \pm E_p$ , which are given by

$$R_+ = \frac{e^{-iE_p z_0}}{2E_p}, \quad R_- = -\frac{e^{iE_p z_0}}{2E_p}. \quad (2.82)$$

To arrive at the Feynman propagator, we must integrate slightly below and above the  $p^0$  axis for  $\text{Re } p^0 < 0$  and  $\text{Re } p^0 > 0$ , respectively (see Fig. 2.1). For  $z_0 > 0$ , we close the contour in the lower half plane (because the integral at infinity vanishes only below) and pick up the positive energy pole. For  $z_0 < 0$ , we close the contour in the upper half plane and pick up the negative energy pole, so the  $p^0$  integral becomes

$$\int dp_0 \frac{e^{-ip_0 z_0}}{p_0^2 - E_p^2} = 2\pi i [-\Theta(z_0) R_+ + \Theta(-z_0) R_-], \quad (2.83)$$

where the positive residue comes with a minus because of the opposite integration direction. In total, the Feynman propagator ‘propagates positive energies forward in time and negative energies backwards’:

$$\begin{aligned} D_F(z) &= \int \frac{d^3 p}{(2\pi)^4} e^{i\mathbf{p} \cdot \mathbf{z}} i(2\pi i) [-\Theta(z_0) R_+ + \Theta(-z_0) R_-] \\ &= \int \frac{d^3 p}{2E_p} \frac{\Theta(z_0) e^{-ipz} + \Theta(-z_0) e^{ipz}}{(2\pi)^3} \Big|_{p^0=E_p} \\ &\stackrel{(2.72)}{=} \Theta(z^0) D(z) + \Theta(-z^0) D(-z), \end{aligned} \quad (2.84)$$

and we see that this is indeed the definition of the Feynman propagator in Eq. (2.76). Note that instead of deforming the integration path in  $p^0$  we could have equally shifted the poles by  $\pm E_p \rightarrow \pm E'_p = \pm(E_p - i\epsilon/(2E_p))$ , as indicated in Fig. 2.1:

$$\frac{1}{p_0^2 - E_p^2} \rightarrow \frac{1}{p_0^2 - E'_p{}^2} = \frac{1}{p_0^2 - E_p^2 + i\epsilon} = \frac{1}{p^2 - m^2 + i\epsilon}, \quad (2.85)$$

so we can equivalently write the Feynman propagator as

$$D_F(z) = \int \frac{d^4 p}{(2\pi)^4} e^{-ipz} \frac{i}{p^2 - m^2 + i\epsilon}. \quad (2.86)$$

Later we will see that this ‘ $i\epsilon$  prescription’ follows from the imaginary-time boundary conditions when projecting Green functions onto the interacting vacuum, which is why it is really the *Feynman* propagator that appears in the interacting quantum field theory (and not any of the other options in performing the contour integral).

**Retarded and advanced propagators.** For completeness we discuss two other physically relevant integration paths. One is to integrate slightly above *both* poles and the other is to integrate slightly below them (see Fig. 2.1). In the first case, for  $z^0 > 0$  we must close the contour in the lower half plane (which gives the sum of the residues) and for  $z^0 < 0$  in the upper half plane (which gives zero); the situation is reversed in the second case. The resulting propagators are the *retarded* and *advanced* propagators:

$$\begin{aligned} D_{R,A}(z) &= \mp \int \frac{d^3 p}{(2\pi)^4} e^{i\mathbf{p}\cdot\mathbf{z}} i(2\pi i) \Theta(\pm z^0) (R_+ + R_-) \\ &= \pm \Theta(\pm z^0) \int \frac{d^3 p}{2E_p} \frac{e^{-ipz} - e^{ipz}}{(2\pi)^3} \Big|_{p^0=E_p} \\ &= \pm \Theta(\pm z^0) (D(z) - D(-z)) = \pm \Theta(\pm z^0) \Delta(z). \end{aligned} \quad (2.87)$$

The retarded propagator has only support in the forward light cone and the advanced propagator in the backward light cone. They also appear in classical field theory in the context of constructing solutions to the inhomogeneous Klein-Gordon equation, where they propagate the inhomogeneity forward ( $D_R$ ) and backward ( $D_A$ ) in time. The classical version of causality states that  $D_R$  and  $D_A$  vanish if  $(x-y)^2 < 0$ , which we also proved here. By contrast, the Feynman propagator  $D_F$  has no classical counterpart. It does not vanish for spacelike distances but rather falls off exponentially outside the light cone.