# Chapter 10 Relativistic Wave Equations

### **10.1 The Relativistic Wave Equation**

In the previous chapter we have recalled the basic notions of non-relativistic quantum mechanics. We have seen that, in the Schroedinger representation, the physical state of a free particle of mass *m* is described by a wave function  $\psi(\mathbf{x}, t)$  which is itself a *classical field* having a probabilistic interpretation. For a single free particle this function is solution to the Schroedinger equation (9.79). A system of *N* interacting particles will be described by a wave function  $\psi(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N; t)$  whose squared modulus represents the probability density of finding the particles at the points  $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N$  at the time *t*. In this description *the number N of particles is always constant* that is it cannot vary during the interaction. Note that the conservation of the number of particles is related to the conservation of mass in a nonrelativistic theory: The sum of the rest masses of the particles cannot change during the interaction. A change in this number would imply a variation in the sum of the corresponding rest masses.

Strictly related to this property of the Schroedinger equation is the fact that the total probability is conserved in time. Let us recall the argument in the case of a single particle.

The normalization of  $\psi(\mathbf{x}, t)$  is fixed by requiring that the probability of finding the particle anywhere in space at any time *t* be one:

$$\int_{V} d^3 \mathbf{x} |\psi(\mathbf{x}, t)|^2 = 1,$$

where  $V = \mathbb{R}^3$  representing the whole space. This total probability should not depend on time, and indeed, by using Schroedinger's equation and Gauss' law we find:

$$\frac{d}{dt} \int_{V} d^{3} \mathbf{x} |\psi(\mathbf{x}, t)|^{2} = \int_{V} d^{3} \mathbf{x} \left( \psi^{*} \frac{\partial}{\partial t} \psi + \psi \frac{\partial}{\partial t} \psi^{*} \right) 
= \frac{i\hbar}{2m} \int_{V} d^{3} \mathbf{x} \left[ (\nabla^{2} \psi) \psi^{*} - \psi \nabla^{2} \psi^{*} \right] 
= \frac{i\hbar}{2m} \int_{V} d^{3} \mathbf{x} \nabla \cdot \left( \psi^{*} \nabla \psi - \psi \nabla \psi^{*} \right) 
= \frac{i\hbar}{2m} \int_{S_{\infty}} dS \mathbf{n} \cdot \left( \psi^{*} \nabla \psi - \psi \nabla \psi^{*} \right) = 0, \quad (10.1)$$

**n** being the unit vector orthogonal to dS and  $S_{\infty}$  is the surface at infinity which ideally encloses the whole space V. The last integral over  $S_{\infty}$  in the above equation then vanishes since both  $\psi$  and  $\nabla \psi$  vanish sufficiently fast at infinity. Thus *the total probability is conserved in time*.

Equation (10.1) can also be neatly expressed, in a local form, as a *continuity equation:* 

$$\partial_t \rho + \nabla \cdot \mathbf{j} = 0, \quad \rho \equiv |\psi(\mathbf{x}, t)|^2, \quad \mathbf{j} \equiv \frac{i\hbar}{2m} (\psi \nabla \psi^* - \psi^* \nabla \psi), \quad (10.2)$$

which, as we have seen, holds by virtue of Schroedinger's equation.

Can the above properties still be valid in a relativistic theory? Let us give some physical arguments about why the very concept of wave function looses its meaning in the context of a relativistic theory. As emphasized in Chap. 9, in non-relativistic quantum mechanics  $\mathbf{x}$  and t play a different role, the former being a dynamical variable as opposed to the latter.

Furthermore we know that one of the most characteristic features of elementary particles is their possibility of generation, annihilation, and reciprocal transformation as a consequence of their interaction. Photons can be generated by electrons in motion within atoms, neutrinos are emitted in  $\beta$ -decays, a neutral pion, a composite particle of a quark and an anti-quark, can decay and produce two photons, a fast electron moving close to a nucleus can produce photons which in turn may transform in electron-positron pairs, and so on.

That means that in phenomena arising from high energy particle interactions, *the number of particles is no longer conserved*.

Consequently some concepts of the non-relativistic formulation of quantum mechanics must be consistently revised.

First of all, we must give up the possibility of localizing in space and time a particle with absolute precision, which was instead allowed in the non-relativistic theory. Indeed if in a relativistic theory we were to localize a particle within a domain of linear dimensions  $\Delta x$  less than  $\hbar/2mc$ , by virtue of the Heisenberg uncertainty principle  $\Delta x \Delta p_x \ge \hbar/2$ , the measuring instrument should exchange with the particle a momentum  $\Delta p_x \ge mc$ , carried for example by a photon. Such a photon of momentum  $\Delta p_x$ , would carry an energy  $\Delta E = c \Delta p_x \ge mc^2$  which is greater than

or equal to the rest energy of the particle. This would be in principle sufficient to create a particle (or better a couple particle-antiparticle, as we shall see) of rest mass m which may be virtually undistinguishable from the original one.

It is therefore impossible to localize a particle in a region whose linear size is of the order of the Compton wavelength  $\hbar/mc$ . In the case of photons, having m = 0 and v = c, the notion of position of the particle simply does not exist.

The existence of a minimal uncertainty  $\Delta x \approx \hbar/mc$  in the position of a particle also implies a basic uncertainty in time, since from the inequality  $\Delta t \Delta E \geq \frac{\hbar}{2}$ and the condition  $\Delta E \leq mc^2 \approx \frac{\hbar c}{\Delta x}$  deduced above, it follows that  $\Delta t \gtrsim \frac{\hbar}{\Delta E} \gtrsim \frac{\Delta x}{c} \approx \hbar/mc^2$  (note that in the non-relativistic theory  $c = \infty$  so that  $\Delta t$  can be zero). As far as the uncertainty in the momentum of a particle is concerned, we note that from  $\Delta x \lesssim c \Delta t$  it follows that  $\Delta p \gtrsim \frac{\hbar}{c\Delta t}$ , that is the uncertainty in the momentum  $p_x$  can be made as small as we wish ( $\Delta p_x \to 0$ ) just by waiting for a sufficiently long time ( $\Delta t \to \infty$ ). This can certainly be done for *free particles*. Localizing a particle in space and time with indefinite precision is thus conceptually not possible within a relativistic context and the interpretation of  $\rho \equiv |\psi(\mathbf{x}, t)|^2$  as the probability density of finding a particle in  $\mathbf{x}$  at a time t should be substantially reconsidered. By the same token, we can conclude that, using the momentum representation  $\tilde{\psi}(\mathbf{p})$  of the wave function instead, we can consistently define a *probability density in the momentum space* as  $|\tilde{\psi}(\mathbf{p})|^2$ .

The argument given above relies on the possibility, in high energy processes, for particles to be created and destroyed. This fact, as anticipated earlier, is at odds with the Schroedinger's formulation of quantum mechanics, which is based on the notion of single particle state, or, in general of multi-particle states with a fixed number of particles. Such description is no longer appropriate in a relativistic theory.

In order to have a more quantitative understanding of this state of affairs let us go back to the quantum description of the electromagnetic field given in Chap. 6.

We have seen that in the Coulomb gauge  $(A^0 = 0, \nabla \cdot \mathbf{A} = 0)$ , the *classical field*  $\mathbf{A}(\mathbf{x}, t)$  satisfies the Maxwell equation:

$$\Box \mathbf{A} = \frac{1}{c^2} \frac{\partial^2}{\partial t^2} \mathbf{A} - \nabla^2 \mathbf{A} = 0.$$
(10.3)

Suppose that we do not quantize the field as we did in Chap. 6, but consider the Maxwell equation as the wave equation for the classical field  $\mathbf{A}(\mathbf{x}, t)$ , just as the Schroedinger equation is the wave equation of the classical field  $\psi(\mathbf{x}, t)$ . We may ask whether a solution  $\mathbf{A}(\mathbf{x}, t)$  to Maxwell's equations can be consistently given the same probabilistic interpretation as a solution  $\psi(\mathbf{x}, t)$  to the Schroedinger equation. In other words, does the quantity  $|A_{\mu}(\mathbf{x}, t)|^2 d^3 \mathbf{x}$  make sense as probability of finding a photon with a given polarization in a small neighborhood  $d^3 \mathbf{x}$  of a point  $\mathbf{x}$  at a time t?

To answer this question we consider the Fourier expansion of the classical field  $A(\mathbf{x}, t)$  given in (6.15):

$$\mathbf{A}(\mathbf{x},t) = \sum_{k_1 k_2 k_3} \left( \boldsymbol{\epsilon}_{\mathbf{k}} e^{-ik \cdot x} + \boldsymbol{\epsilon}_{\mathbf{k}}^* e^{ik \cdot x} \right), \qquad (10.4)$$

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where  $\epsilon_{\mathbf{k}}$  can be written as in (6.42)

$$\boldsymbol{\epsilon}_{\mathbf{k}} = c \sqrt{\frac{\hbar}{2\omega_k V}} \sum_{\alpha=1}^2 a_{\mathbf{k},\alpha} \mathbf{u}_{\mathbf{k},\alpha}, \qquad (10.5)$$

but with the operators  $a, a^{\dagger}$  replaced by numbers  $a, a^{*}$  since we want to consider  $A(\mathbf{x}, t)$  as a *classical* field. If Maxwell's propagation equation could be regarded as a quantum wave equation, then, according to ordinary quantum mechanics, the (complex) component of the Fourier expansion of  $A(\mathbf{x}, t)$ 

$$\mathbf{A}_{\mathbf{k},\alpha}(x) \equiv c_{\sqrt{\frac{\hbar}{2\omega_{k}V}}} a_{\mathbf{k},\alpha} \mathbf{u}_{\mathbf{k},\alpha} e^{-ik \cdot x},$$

can be given the interpretation of *eigenstate* of the four momentum operator  $\hat{P}_{\mu}$ , describing a free particle with polarization  $\mathbf{u}_{\mathbf{k},\alpha}$ , energy  $E = \hbar \omega$  and momentum  $\mathbf{p} = \hbar \mathbf{k}$ , respectively and satisfying the relation  $E/c = |\mathbf{p}|$ . This would imply that  $\mathbf{A}_{\mathbf{k},\alpha}(x)$  represents the wave function of a *photon* with definite values of energy and momentum. Consequently it would seem reasonable to identify the four potential  $A_{\mu}(\mathbf{x}, t)$  as the *photon wave function* expanded in a set of eigenstates, so that the Maxwell equation for the vector potential would be the natural relativistic generalization of the non-relativistic Schroedinger's equation.

We note however that, while the Schroedinger's equation is of *first order in the time derivatives*, the Maxwell equation, being relativistic and therefore Lorentz invariant, contains the operator  $\Box \equiv 1/c^2 \partial_t^2 - \nabla^2$  which is of *second order both in time and in spatial coordinates*. This makes a great difference as far as the conservation of probability is concerned since the proof (10.1) of the continuity (10.2) makes use of the Schroedinger equation (9.78). More specifically such proof strongly relies on the fact that the Schroedinger equation is of first order in the time derivative and of second order in the spatial ones.

The fact that Maxwell's propagation equation, involves *second order derivatives* with respect to time, makes it impossible to derive a continuity equation for the "would be" probability density  $\rho \equiv |\mathbf{A}(x)|^2$ :  $\partial_t \rho + \nabla \cdot \mathbf{j} \neq 0$ . Indeed the first order time derivatives are actually Cauchy data of the Maxwell propagation equation. As a consequence *the quantity*  $\rho$  *cannot be interpreted as a probability density, since the total probability of finding a photon in the whole space would not be conserved.* 

On the other hand, as we have illustrated when discussing the quantization of the electromagnetic field, these difficulties are circumvented if we quantize the infinite set of canonical variables associated with  $A_{\mu}(\mathbf{x}, t)$  by the usual prescription of converting Poisson brackets into commutators. This is effected by converting the coefficients  $a_{\mathbf{k},\alpha}$ ,  $a_{\mathbf{k},\alpha}^*$ , defined in (10.5), and thus each Fourier component  $\epsilon_{\mathbf{k}}$ , into operators through the general procedure introduced in Chap. 6 under the name of *second quantization*. In this new framework the classical field  $\mathbf{A}_{\mu}(\mathbf{x}, t)$  becomes a *quantum field*, that is an operator, and the quantum states of the electromagnetic field are described in the *occupation number representation* by the multi-photon state  $|\{N_{\mathbf{k},\alpha}\}\rangle$ , characterized by  $N_{\mathbf{k},\alpha}$  photons in each single-particle state  $(\mathbf{k}, \alpha)$ . We may therefore expect the same considerations to apply, as we shall see, also to *free* particles of spin 0 and 1/2, for which a consistent relativistic description can be achieved by a *quantum field theory* in which particles are seen as quantized excitations of a field, in the same way as photons were defined as quantum excitations of the electromagnetic field.

Notwithstanding the difficulties of interpretation mentioned above, it is however our purpose to give in this chapter, a treatment of the *classical wave equations* for spin 0 and 1/2 particles in some detail for two reasons: First we want to give a precise quantitative discussion of how inconsistencies show up when trying to interpret the relativistic fields as wave functions of one-particle states, thus tracing back the historical development of relativistic quantum theories. Second, the formal development of these equations will allow us to assemble those formulae which we shall need in the next chapter where the "second quantization" of the spin 0 and 1/2 fields will be developed, that is the classical fields will be treated as dynamic variables and, as such, promoted to quantum operators. As shown for the electromagnetic case, the second quantization procedure allows to describe the system in terms of states which differ in the number of particles they describe and thus provides an ideal framework in which to analyze relativistic processes involving the creation and destruction of particles, namely in which the number and the identities of the interacting particles are not conserved. This will be dealt with in Chap. 12, where a relativistically covariant, perturbative description of fields in interaction will be developed for the electromagnetic field in interaction with a Dirac field. This analysis provides however a paradigm for the description of all the other fundamental interactions among elementary particles.

## **10.2 The Klein–Gordon Equation**

Let us consider a relativistic field theory describing a *classical* field  $\Phi^{\alpha}(x^{\mu})$ . Such field is defined by its transformation property (7.47) under a generic Poincaré transformation ( $\Lambda$ ,  $\mathbf{x}_0$ ) (7.46):

$$(\mathbf{\Lambda}, \mathbf{x}_0) : x^{\mu} \to x'^{\mu} = {\mathbf{\Lambda}^{\mu}}_{\nu} x^{\nu} - x_0^{\mu},$$
  
$$\Phi^{\alpha}(x) \to {\Phi'}^{\alpha}(x') = D^{\alpha}{}_{\beta} \Phi^{\beta}(x) = D^{\alpha}{}_{\beta} \Phi^{\beta}(\mathbf{\Lambda}^{-1}(x'+x_0)),$$

where  $\mathbf{D} = (D^{\alpha}{}_{\beta}) = \mathbf{D}(\mathbf{\Lambda})$  represents the action of the Lorentz transformation  $\mathbf{\Lambda}$  on the *internal degrees of freedom* of the field, labeled by  $\alpha$  and defining a representation of the Lorentz group SO(1, 3). In Chaps. 7 and 9, see (9.101), the action of a Poincaré transformation on  $\Phi^{\alpha}(x)$  was described in terms of the infinitesimal generators  $\hat{J}_{\mu\nu}$ associated with the Lorentz part, and  $\hat{P}_{\mu}$  generating space-time translations. The latter provide the operator representation, in a relativistic quantum theory, of the four-momentum of a particle:

$$\hat{P}^{\mu} \equiv \left(\frac{1}{c}\hat{H}, \hat{\mathbf{p}}\right) = i\hbar\eta^{\mu\nu}\partial_{\nu}.$$
(10.6)

The identification of the Hamiltonian operator, function of the particle position and the momentum operator, with the generator of time evolution  $i\hbar\partial_t$  is expressed by the Schroedinger equation (9.78), and describes the dynamics of the system. For a free particle this equation has the form (9.79), which is clearly not Lorentz covariant, since it is obtained from the non-relativistic relation  $E = |\mathbf{p}|^2/2m$  upon replacing

$$\mathbf{p} \to \hat{\mathbf{p}} = -i\hbar \nabla, \quad E \to \hat{H} = i\hbar\partial_t.$$
 (10.7)

In seeking for the simplest Lorentz-covariant generalization of the Schrödinger equation describing a free particle, we should start from the mass-shell condition in relativistic mechanics which relates the linear momentum and the energy with the rest mass of the particle

$$\mathbf{p}^2 + m^2 c^2 = \frac{E^2}{c^2} \longleftrightarrow p^{\mu} p_{\mu} - m^2 c^2 = 0.$$
 (10.8)

Implementing the same canonical prescription (10.7) on  $\Phi^{\alpha}$  we end up with (9.107) of the previous chapter, which can be written in the following compact form:

$$\left(\Box + \frac{m^2 c^2}{\hbar^2}\right) \Phi^{\alpha}(x) = 0.$$
(10.9)

By construction the above equation represents a manifestly *Lorentz invariant* generalization of the Schroedinger equation<sup>1</sup> and is referred to as the *Klein–Gordon* equation.

We note that *this equation should hold for particles of any spin*, that is for any representation of the Lorentz group carried by the index  $\alpha$ . For example, in the case of the electromagnetic field, setting  $\phi^{\alpha}(x) \equiv A_{\mu}(x)$  and m = 0 we obtain

$$\Box A_{\mu}(x) = 0, \tag{10.10}$$

that is the Maxwell propagation equation for the electromagnetic four-potential describing particles of spin 1, in the Lorentz gauge. We shall see in the sequel that also the wave functions of spin 1/2 satisfy the Klein–Gordon equation.

In the rest of this section we shall treat exclusively the case of spin 0 fields, that is fields that are *scalar* under Lorentz transformations. We shall consider a *complex scalar field*,  $\phi$ , or equivalently two real scalar fields (see Chap. 7, Sect. 7.4).

In this case the equation of motion (10.9) can be derived from the Hamilton principle of stationary action, starting from the following Lagrangian density (8.198):

$$\mathcal{L} = c^2 \left( \partial_\mu \phi^* \partial^\mu \phi - \frac{m^2 c^2}{\hbar^2} \phi^* \phi \right).$$
(10.11)

<sup>&</sup>lt;sup>1</sup> Extension of the invariance to the full Poincaré group is obvious.

Indeed in this case the Euler–Lagrange equations

$$\frac{\partial \mathcal{L}}{\partial \phi(x)^*} - \partial_\mu \left( \frac{\partial \mathcal{L}}{\partial \partial_\mu \phi(x)^*} \right) = 0; \quad \frac{\partial \mathcal{L}}{\partial \phi(x)} - \partial_\mu \left( \frac{\partial \mathcal{L}}{\partial \partial_\mu \phi(x)} \right) = 0,$$

give:

$$\left(\Box + \frac{m^2 c^2}{\hbar^2}\right)\phi(x) = 0.$$
(10.12)

together with its complex conjugate.

As a complete set of solutions we can take the plane waves (9.113)

$$\Phi_p(x) \propto e^{-\frac{i}{\hbar}p^{\mu}x_{\mu}},\tag{10.13}$$

with wave number  $\mathbf{k} = \mathbf{p}/\hbar$  and angular frequency  $\omega = E/\hbar$ . These are the eigenfunctions of the operator  $\hat{P}^{\mu}$  which describe the wave functions of particles with definite value of energy *E* and momentum **p**, see Chap. 9. Substituting the exponentials (10.13) in (10.12) we find

$$\frac{E^2}{c^2} - |\mathbf{p}|^2 = m^2 c^2, \qquad (10.14)$$

or

$$E = \pm E_{\mathbf{p}} = \pm \sqrt{|\mathbf{p}|^2 c^2 + m^2 c^4}.$$
 (10.15)

We see that solutions exist for both positive and *negative* values of the energy corresponding to the exponentials:

$$e^{-\frac{i}{\hbar}(E_{\mathbf{p}}t-\mathbf{p}\cdot\mathbf{x})}; \quad e^{\frac{i}{\hbar}(E_{\mathbf{p}}t+\mathbf{p}\cdot\mathbf{x})}.$$
(10.16)

Strictly speaking this is not a problem as long as we consider only *free fields*. Indeed the conservation of energy would forbid transition between positive and negative energy solutions and a positive energy state will remain so. Therefore we could regard as physical only those solutions corresponding to positive energy E > 0. However the very notion of free particle is far from reality since real particles interact with each other, usually in scattering processes. During an interaction transitions between quantum states are induced, according to perturbation theory. Therefore we cannot neglect the existence of negative energy states. For example, a particle with energy  $E = +E_p$  could decay into a particle of energy  $E = -E_p$ , through the emission of a photon of energy  $2E_p$ . Moreover the existence of negative energies is in some sense contradictory since, as shown in the following, from a field theoretical point of view, the Hamiltonian of the theory is *positive definite*.<sup>2</sup>

Thus, the existence of negative energy solutions is a true problem when trying to achieve a relativistic generalization of the Schroedinger equation.

<sup>&</sup>lt;sup>2</sup> Furthermore, erasing the negative energy solutions would spoil the completeness of the eigenstates of  $\hat{P}^{\mu}$  and the expansion in plane waves would be no longer correct.

A second problem arises when trying to give a probabilistic interpretation to the wave function  $\psi(\mathbf{x}, t)$ . As we have anticipated in the introduction with each solution to the Schroedinger equation we can associate a a *positive* probability  $\rho = |\psi(\mathbf{x}, t)|^2$ , and a current density  $\mathbf{j} = \frac{i\hbar}{2m}(\psi\nabla\psi^* - \psi^*\nabla\psi)$  satisfying the *continuity* equation (10.2), which assures that the total probability is conserved.

We can attempt to follow the same route for the Klein–Gordon equation, and associate with its solution a conserved current, i.e. a current  $j^{\mu}$  for which we can write a continuity equation in the form  $\partial_{\mu} j^{\mu} = 0$ . Although this can be done, as we are going to illustrate below, the conserved quantity associated with  $j^{\mu}$  cannot be consistently identified with a total probability. To construct  $j^{\mu}$  let us multiply (10.9) by  $\phi^*$ 

$$\phi^* \left( \Box + \frac{m^2 c^2}{\hbar^2} \right) \phi = 0,$$

and subtract the complex conjugate expression. We obtain:

$$\phi^* \left( \Box + \frac{m^2 c^2}{\hbar^2} \right) \phi - \phi \left( \Box + \frac{m^2 c^2}{\hbar^2} \right) \phi^* = 0,$$

which can be written as a conservation law:

$$\partial_{\mu}j^{\mu}(x) = 0, \tag{10.17}$$

where<sup>3</sup>

$$j^{\mu} = i \left( \phi^* \partial^{\mu} \phi - \partial^{\mu} \phi^* \phi \right).$$
(10.18)

Note however that  $j^0 = \frac{i}{c}(\phi^*\dot{\phi} - \phi\dot{\phi}^*)$  is not positive definite and thus cannot be identified with a probability density. In fact this current has a different physical interpretation. If we define

$$J^{\mu} = \frac{ce}{\hbar} j^{\mu} = \frac{ice}{\hbar} \left( \phi^* \partial^{\mu} \phi - \partial^{\mu} \phi^* \phi \right), \qquad (10.19)$$

we recognize this as the *conserved current* in (8.202), associated with the invariance of the Lagrangian equation (10.11) under the symmetry transformation (8.200). The corresponding conserved Noether charge was given by (8.203), namely:

$$Q = \int d^3 \mathbf{x} J^0 = i \frac{e}{\hbar} \int d^3 \mathbf{x} (\phi^* \partial_t \phi - \phi \partial_t \phi^*), \qquad (10.20)$$

and was interpreted in Chap. 8 as the charge carried by a complex field.<sup>4</sup>

<sup>&</sup>lt;sup>3</sup> The factor i has been inserted in order to have a *real* current.

<sup>&</sup>lt;sup>4</sup> Actually this "charge" can be any conserved quantum number associated with invariance under U(1) transformations, like baryon or lepton number etc. However we will always refer to the *electric charge*.

Notwithstanding the above difficulties we shall develop in the following all the properties of the Klein–Gordon equation since they will be very useful in the second quantized version of the scalar field theory.

Let us now write down the *most general* solution to the Klein–Gordon equation. It can be written in a form in which relativistic invariance is manifest:

$$\phi(x) = \frac{1}{(2\pi\hbar)^3} \int d^4 p \tilde{\phi}(p) \delta(p^2 - m^2 c^2) e^{-\frac{i}{\hbar}p \cdot x}$$
(10.21)

where  $d^4 p = dp^0 d^3 \mathbf{p}$ . Let us comment on this formula. We have first solved (10.12), as we did for Maxwell's equation in the vacuum (5.96), in a finite size box of volume *V*, see Sect. 5.6, so that the momenta of the solutions have *discrete* values  $\mathbf{p} = \hbar \mathbf{k} = \hbar \left(\frac{2\pi n_1}{L_A}, \frac{2\pi n_2}{L_B}, \frac{2\pi n_3}{L_C}\right)$  as a consequence of the *periodic boundary conditions* on the box. We have then considered the large volume limit  $V \to \infty$ , see Sect. 5.6.2, in which the components of the linear momentum become continuous variables and the discrete sum over  $\mathbf{p}$  is replaced by a triple integral, according to the prescription (5.121):

$$\sum_{\mathbf{p}} \to \frac{V}{(2\pi\hbar)^3} \int d^3 \mathbf{p}.$$
 (10.22)

This explains the factor  $1/(2\pi\hbar)^3$  in (10.21) while the normalization volume V has been absorbed in the definition of  $\tilde{\phi}(p)$ . Secondly, the Dirac delta function  $\delta(p^2 - m^2c^2)$  makes the integrand non-zero only for  $p^0 = \frac{E}{c} = \pm \frac{E_p}{c}$ , thus implementing condition (10.15). Indeed, applying the Klein–Gordon operator to (10.21) and using the property  $x\delta(x) = 0$  we find:

$$\left(\Box + \frac{m^2 c^2}{\hbar^2}\right)\phi(x) \propto \int d^4 p \tilde{\phi}(p) (-p^2 + m^2 c^2) \delta(p^2 - m^2 c^2) e^{-\frac{i}{\hbar}p \cdot x} = 0,$$
(10.23)

that is the Klein–Gordon equation is satisfied by the expression (10.21).

The representation (10.21) of the general solution of the Klein–Gordon equation has the advantage of being explicitly Lorentz invariant, but it is not very manageable. A more convenient representation is found by eliminating the constraint implemented by the delta function. This can be done by integrating over  $p^0$  so that only the integration on  $d^3\mathbf{p}$  remains.

For this purpose we recall the following property of the Dirac delta function: Given a function f(x) with a certain number *n* of *simple* zeros,  $f(x_i) = 0, x_i$ , (i = 1, ..., n), then

$$\delta(f(x)) = \sum_{i=1}^{n} \frac{1}{|f'(x_i)|} \delta(x - x_i).$$
(10.24)

We apply this formula to the function  $f(E) = p^2 - m^2 c^2 = \frac{E^2}{c^2} - |\mathbf{p}|^2 - m^2 c^2$ . It has two simple zeros corresponding to  $E = \pm E_{\mathbf{p}}$ . Taking into account that

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$$|f'(\pm E_{\mathbf{p}})| = \frac{2}{c^2} E_{\mathbf{p}},$$
(10.25)

the derivative being computed with respect to E, and using (10.24), we find:

$$\delta(p^2 - m^2 c^2) = \frac{c^2}{2E_{\mathbf{p}}} \left( \delta(E - E_{\mathbf{p}}) + \delta(E + E_{\mathbf{p}}) \right).$$
(10.26)

Substituting this expression in (10.21) one obtains:

$$\begin{split} \phi(\mathbf{x}) &= \frac{c}{(2\pi\hbar)^3} \int d^3 \mathbf{p} \int \frac{dE}{2E_{\mathbf{p}}} \tilde{\phi}(p) \left( \delta(E - E_{\mathbf{p}}) + \delta(E + E_{\mathbf{p}}) e^{-\frac{i}{\hbar} \mathbf{p} \cdot \mathbf{x}} \right) \\ &= \frac{c}{(2\pi\hbar)^3} \int \frac{d^3 \mathbf{p}}{2E_{\mathbf{p}}} \left( \tilde{\phi}(E_{\mathbf{p}}, \mathbf{p}) e^{-\frac{i}{\hbar}(E_p t - \mathbf{p} \cdot \mathbf{x})} \right. \\ &+ \tilde{\phi}(-E_{\mathbf{p}}, -\mathbf{p}) e^{-\frac{i}{\hbar}(-E_p t - (-\mathbf{p}) \cdot \mathbf{x})} \right). \end{split}$$
(10.27)

Note that in the second term of the integrand we have replaced the integration variable **p** with  $-\mathbf{p}$ ; such change is immaterial since the integration in  $d^3\mathbf{p}$  runs over all the directions of **p**. This replacement however allows us to rewrite the argument of the exponential  $e^{-\frac{i}{\hbar}(-E_pt-(-\mathbf{p})\cdot\mathbf{x})}$  as  $\frac{i}{\hbar}$  times the product of the four-vectors  $p^{\mu} = (\frac{1}{c}E_{\mathbf{p}}, \mathbf{p})$  and  $x^{\mu}$ :

$$e^{-\frac{i}{\hbar}(-E_pt-(-\mathbf{p})\cdot\mathbf{x})} = e^{\frac{i}{\hbar}(E_pt-\mathbf{p}\cdot\mathbf{x})} = e^{\frac{i}{\hbar}p\cdot\mathbf{x}}.$$
(10.28)

Thus (10.27) takes the final form:

$$\phi(x) = \frac{c}{(2\pi\hbar)^3} \int \frac{d^3\mathbf{p}}{2E_p} \left[ \tilde{\phi}_+(p) e^{-\frac{i}{\hbar}p \cdot x} + \tilde{\phi}_-(p) e^{\frac{i}{\hbar}p \cdot x} \right] = \frac{1}{(2\pi\hbar)^3} \int \frac{d^3\mathbf{p}}{2p^0} \left[ \tilde{\phi}_+(p) e^{-\frac{i}{\hbar}p \cdot x} + \tilde{\phi}_-(p) e^{\frac{i}{\hbar}p \cdot x} \right],$$
(10.29)

where  $p^0 \equiv E_{\mathbf{p}}/c$  and we have defined

$$\tilde{\phi}_{+}(p) \equiv \tilde{\phi}(E_{\mathbf{p}}, \mathbf{p}); \quad \tilde{\phi}_{-}(p) \equiv \tilde{\phi}(-E_{\mathbf{p}}, -\mathbf{p}).$$
(10.30)

They represent the Fourier transforms of the positive and negative energy solutions.

It is important to note that in the particular case of a *real* field  $\phi(x)$ ,  $\phi(x) = \phi^*(x)$ , the two Fourier coefficients would be related by complex conjugation,  $\tilde{\phi}^*_+ = \tilde{\phi}_-$ . Instead in the present case of a complex scalar field there is no relation between them. We also note, by comparing (10.21) and (10.29), that *the quantity*  $\frac{d^3\mathbf{p}}{2E_{\mathbf{p}}}$  is Lorentz invariant (see also Sect. 9.5). In summary (10.29) represents the most general solution of the Klein–Gordon equation for a complex scalar field  $\phi(x)$ , given

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in terms of both positive and negative energy solutions. Moreover (10.29), though not manifestly, is *Lorentz invariant* since it has been derived from (10.21).

For future purpose it is interesting to compute the conserved charge (10.20) in terms of the Fourier coefficients (10.30).

To this end let us first compute the Fourier integral form of  $\dot{\phi}(x)$  from (10.29):

$$\dot{\phi}(x) = -ic \int \frac{d^3 \mathbf{p}}{2(2\pi\hbar)^3\hbar} \left[ \tilde{\phi}_+(p) e^{-\frac{i}{\hbar}p \cdot x} - \tilde{\phi}_-(p) e^{\frac{i}{\hbar}p \cdot x} \right].$$
(10.31)

Inserting the general solution (10.29) and (10.31) in the left hand side of the following equation:

$$\frac{\hbar}{e}Q = i \int d^3 \mathbf{x} (\phi^* \dot{\phi}) + c.c.$$

we find a number of terms involving two momentum and one volume integrals. The integral in  $d^3x$  can be performed over the exponentials and yields delta functions according to the property:

$$\int d^3 \mathbf{x} e^{\pm \frac{i}{\hbar} (\mathbf{p} - \mathbf{p}') \cdot \mathbf{x}} = (2\pi\hbar)^3 \delta^3 (\mathbf{p} - \mathbf{p}').$$
(10.32)

Let us consider each term separately. The terms containing the products  $\phi_+\phi_+$  give the following contribution:

$$\frac{c}{(2\pi\hbar)^6} \int d^3 \mathbf{x} \int \frac{d^3 \mathbf{p}}{4\hbar p_0} \int d^3 \mathbf{q} \left[ \tilde{\phi}_+^*(p) \tilde{\phi}_+(q) e^{+\frac{i}{\hbar}((p_0-q_0)x_0-(\mathbf{p}-\mathbf{q}))\cdot\mathbf{x}} + c.c. \right] \\
= \frac{c}{(2\pi\hbar)^3} \int \frac{d^3 \mathbf{p}}{4\hbar p_0} \int d^3 \mathbf{q} \left[ \tilde{\phi}_+^*(p) \tilde{\phi}_+(q) e^{+\frac{i}{\hbar}(p_0-q_0)x_0} \delta^3(\mathbf{p}-\mathbf{q}) + c.c. \right] \\
= \frac{c}{(2\pi\hbar)^3} \int \frac{d^3 \mathbf{p}}{4\hbar p_0} \left[ \tilde{\phi}_+^*(p) \tilde{\phi}_+(p) + c.c. \right] = \frac{c}{(2\pi\hbar)^3\hbar} \int \frac{d^3 \mathbf{p}}{2p_0} \tilde{\phi}_+^*(p) \tilde{\phi}_+(p).$$

where we have used the fact that if  $\mathbf{p} = \mathbf{q}$ , then  $E_{\mathbf{p}} = E_{\mathbf{q}}$ . Similarly, for the  $\phi_{-}\phi_{-}$  terms we find:

$$-\frac{c}{(2\pi\hbar)^6}\int d^3\mathbf{x}\int \frac{d^3\mathbf{p}}{4\hbar p_0}\int d^3\mathbf{q}\tilde{\phi}_-^*(p)\tilde{\phi}_-(q)e^{-\frac{i}{\hbar}((p_0-q_0)x_0-(\mathbf{p}-\mathbf{q}))\cdot\mathbf{x}}+c.c.$$
$$=-\frac{c}{(2\pi\hbar)^3}\int \frac{d^3\mathbf{p}}{2\hbar p_0}\tilde{\phi}_-^*(p)\tilde{\phi}_-(p).$$

Finally the terms containing the mixed products  $\phi_+\phi_-$  give a vanishing contribution:

$$\begin{aligned} \frac{c}{(2\pi\hbar)^6} \int d^3 \mathbf{x} \int \frac{d^3 \mathbf{p}}{4\hbar p_0} \int d^3 \mathbf{q} \left[ \tilde{\phi}_-^*(p) \tilde{\phi}_+(q) e^{-\frac{i}{\hbar}((p_0+q_0)x_0-(\mathbf{p}+\mathbf{q}))\cdot \mathbf{x}} - \tilde{\phi}_+^*(p) \tilde{\phi}_-(q) e^{\frac{i}{\hbar}((p_0+q_0)x_0-(\mathbf{p}+\mathbf{q}))\cdot \mathbf{x}} \right] + c.c. \\ = \frac{c}{(2\pi\hbar)^3} \int \frac{d^3 \mathbf{p}}{4\hbar p_0} \left[ \tilde{\phi}_-^*(p_0,\mathbf{p}) \tilde{\phi}_+(p_0,-\mathbf{p}) e^{-\frac{2i}{\hbar}p_0x_0-(p_0,\mathbf{p})} - \tilde{\phi}_+^*(p_0,-\mathbf{p}) \tilde{\phi}_-(p_0,\mathbf{p}) e^{\frac{2i}{\hbar}p_0x_0} \right] + c.c. = 0. \end{aligned}$$

The last equality is due to the fact that the expression within brackets, being the difference between two complex conjugate terms, is purely imaginary and therefore, when adding to it its own complex conjugate, we obtain zero. The final result is therefore:

$$Q = \frac{1}{(2\pi\hbar)^3} \frac{ec}{\hbar^2} \int \frac{d^3\mathbf{p}}{2p_0} \left[ \tilde{\phi}_+^*(p)\tilde{\phi}_+(p) - \tilde{\phi}_-^*(p)\tilde{\phi}_-(p) \right]$$
(10.33)

confirming the fact that Q is not a positive definite quantity.

In the introduction we have pointed out that the difficulties in giving a probabilistic interpretation to wave functions satisfying a relativistic equation is ultimately related to the fact that in the relativistic processes the number and identities of the particles involved is not conserved. We also know, however, that in any experiment performed so far, the *electric charge is always conserved*. We may therefore argue that the conserved quantity Q should be interpreted as the *total charge* and  $J^0$  as the charge density. Furthermore, from (10.33), it follows that solutions with positive and negative energy have *opposite charge*. This will have a consistent physical interpretation only when, in next chapter, we shall pursue the second quantization program and promote the field  $\phi(x)$  to a quantum operator acting on multi-particle states. The quantity Q will be reinterpreted as the *charge operator* and the positive and negative energy solutions will describe the creation and destruction on a state of positive energy solutions associated with *particles* and *antiparticles* having opposite charge.

Note that a real field has charge  $Q \equiv 0$ , since  $\phi_- = \phi_+^*$ , so that it must describe a *neutral particle* coinciding with its own antiparticle. This is the case, for example, of the electromagnetic field.

# 10.2.1 Coupling of the Complex Scalar Field $\phi(x)$ to the Electromagnetic Field

We show in this section that the charge Q introduced in the previous section can be given the interpretation of *electric charge* carried by the particle whose wave function is described by a *complex scalar field*. To this end, we observe that the presence of electric charge can only be ascertained by letting the particle interact with an