Relativistic Quantum Mechanics

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Springer

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ISSN 1864-5879 e-ISSN 1864-5887
ISBN 978-90-481-3644-5 e-ISBN 978-90-481-3645-2
DOI 10.1007/978-90-481-3645-2

Library of Congress Control Number: 2010928392

Printed on acid-free paper

Springer is part of Springer Science+Business Media (www.springer.com)

Preface

It is more important to repair errors than to prevent them. This is the quintessence of the philosophy of human cognition known as critical rationalism which is perhaps at its most dominant in modern natural sciences. According to it insights are gained through a series of presumptions and refutations, through preliminary solutions that are continuously, rigorously, and thoroughly tested. Here it is of vital importance that insights are never verifiable but, at most, falsifiable. In other words: a natural scientific theory can at most be regarded as "not being demonstrably false" until it can be proven wrong. By contrast, a sufficient criterion to prove its correctness does not exist.

Newtonian mechanics, for example, could be regarded as "not being demonstrably false" until experiments with the velocity of light were performed at the end of the 19th century that were contradictory to the predictions of Newton's theory. Since, so far, Albert Einstein's theory of special relativity does not contradict physical reality (and this theory being simple in terms of its underlying assumptions), relativistic mechanics is nowadays regarded as the legitimate successor of Newtonian mechanics. This does not mean that Newton's mechanics has to be abandoned. It has merely lost its fundamental character as its range of validity is demonstrably restricted to the domain of small velocities compared to that of light.

In the first decade of the 20th century the range of validity of Newtonian mechanics was also restricted with regard to the size of the physical objects being described. At this time, experiments were carried out showing that the behavior of microscopic objects such as atoms and molecules is totally different from the predictions of Newton's theory. The theory more capable of describing these new phenomena is nonrelativistic quantum mechanics and was developed in the subsequent decade. However, already at the time of its formulation, it was clear that the validity of this theory is also restricted as it does not respect the principles of special relativity.

Today, about one hundred years after the advent of nonrelativistic quantum mechanics, it is *quantum field theories* that are regarded as "not being demonstrably false" for the description of microscopic natural phenomena.

They are characterized by the facts that

- they can be Lorentz-covariantly formulated, thus being in agreement with special relativity
- they are many-particle theories with infinitely many degrees of freedom and account very precisely for particle creation and annihilation processes.

Naturally, the way toward these modern theories proceeded through some intermediate steps. One began with nonrelativistic quantum mechanics – in conjunction with its one-particle interpretation – and tried to extend this theory in such a way that it becomes Lorentz-covariant. This initially led to the *Klein-Gordon equation* as a relativistic description of spin-0 particles. However, this equation contains a basic flaw because it leads to solutions with negative energy. Apart from the fact that they seem to have no reasonable interpretation, their existence implies quantum mechanically that stable atoms are not possible as an atomic electron would fall deeper and deeper within the unbounded negative energy spectrum via continuous radiative transitions. Another problem of this equation is the absence of a positive definite probability density which is of fundamental importance for the usual quantum mechanical statistical interpretation. These obstacles are the reason that for a long time, the Klein-Gordon equation was not believed to be physically meaningful.

In his efforts to adhere to a positive definite probability density, Dirac developed an equation for the description of electrons (more generally: spin-1/2 particles) which, however, also yields solutions with negative energy. Due to the very good accordance of Dirac's predictions with experimental results in the low energy regime where negative energy solutions can be ignored (e.g. energy spectrum of the hydrogen atom or gyromagnetic ratio of the electron), it was hardly possible to negate the physical meaning of this theory completely.

In order to prevent electrons from falling into negative energy states, Dirac introduced a trick, the so-called *hole theory*. It claims that the vacuum consists of a completely occupied "sea" of electrons with negative energy which, due to Pauli's exclusion principle, cannot be filled further by a particle. Additionally, this novel assumption allows for an (at least qualitatively acceptable) explanation of processes with changing particle numbers. According to this, an electron with negative energy can absorb radiation, thus being excited into an observable state of positive energy. In addition, this electron leaves a hole in the sea of negative energies indicating the absence of an electron with negative energy. An observer relative to the vacuum interprets this as the presence of a particle with an opposite charge and opposite (i.e. positive) energy. Obviously, this process of *pair creation* implies that, besides the electron, there must exist another particle which distinguishes itself from the electron just by its charge. This particle, the so-called *positron*, was indeed found a short time later and provided an impressive confirmation of Dirac's ideas. Today it is well-known that for each particle there exists an antiparticle with opposite (not necessarily electric) charge quantum numbers.

The problem of the absence of a positive definite probability density could finally be circumvented in the Klein-Gordon theory by interpreting the quantities ρ and $\boldsymbol{j}$ as charge density and charge current density (*charge interpretation*). However, in this case, the transition from positive into negative energy states could not be eliminated in terms of the hole theory, since Pauli's exclusion principle does not apply here and, therefore, a completely filled sea of spin-0 particles with negative energy cannot exist.

The Klein-Gordon as well as the Dirac theory provides experimentally verifiable predictions as long as they are restricted to low energy phenomena where particle creation and annihilation processes do not play any role. However, as soon as one attempts to include high energy processes both theories exhibit deficiencies and contradictions. Today the most successful resort is – due to the absence of contradictions with experimental results – the transition to quantized fields, i.e. to quantum field theories.

This book picks out a certain piece of the cognitive process just described and deals with the theories of Klein, Gordon, and Dirac for the relativistic description of massive, electromagnetically interacting spin-0 and spin-1/2 particles excluding quantum field theoretical aspects as far as possible (relativistic quantum mechanics "in the narrow sense"). Here the focus is on answering the following questions:

- How far can the concepts of nonrelativistic quantum mechanics be applied to relativistic quantum theories?
- Where are the limits of a relativistic one-particle interpretation?
- What similarities and differences exist between the Klein-Gordon and Dirac theories?
- How can relativistic scattering processes, particularly those with pair creation and annihilation effects, be described using the Klein-Gordon and Dirac theories without resorting to the formalism of quantum field theory and where are the limits of this approach?

Unlike many books where the "pure theories" of Klein, Gordon, and Dirac are treated very quickly in favor of an early introduction of field quantization, the book in hand emphasizes this particular viewpoint in order to convey a deeper understanding of the accompanying problems and thus to explicate the necessity of quantum field theories.

This textbook is aimed at students of physics who are interested in a concisely structured presentation of relativistic quantum mechanics "in the narrow sense" and its separation from quantum field theory. With an emphasis on comprehensibility and physical classification, this book ranges on a middle mathematical level and can be read by anybody who has attended theoretical courses of classical mechanics, classical electrodynamics, and nonrelativistic quantum mechanics.

This book is divided into three chapters and an appendix. The first chapter presents the Klein-Gordon theory for the relativistic description of spin-0 particles. As mentioned above, the focus lies on the possibilities and limits of its one-particle interpretation in the usual nonrelativistic quantum mechanical sense. Additionally, extensive symmetry considerations of the Klein-Gordon theory are made, its nonrelativistic approximation is developed systematically in powers of v/c, and, finally, some simple one-particle systems are discussed.

In the second chapter we consider the Dirac theory for the relativistic description of spin-1/2 particles where, again, emphasis is on its one-particle interpretation. Both theories, emanating from certain enhancements of nonrelativistic quantum mechanics, allow for a very direct one-to-one comparison of their properties. This is reflected in the way that the individual sections of this chapter are structured like those of the first chapter – of course, apart from Dirac-specific issues, e.g. the hole theory or spin that are considered separately.

The third chapter covers the description of relativistic scattering processes within the framework of the Dirac and, later on, Klein-Gordon theory. In analogy to nonrelativistic quantum mechanics, relativistic propagator techniques are developed and considered together with the well-known concepts of scattering amplitudes and cross sections. In this way, a scattering formalism is created which enables one-particle scatterings in the presence of electromagnetic background fields as well as two-particle scatterings to be described approximately. Considering concrete scattering processes to lowest orders, the Feynman rules are developed putting all necessary calculations onto a common ground and formalizing them graphically. However, it is to be emphasized that these rules do not, in general, follow naturally from our scattering formalism. Rather, to higher orders they contain solely quantum field theoretical aspects. It is exactly here where this book goes for the first time beyond relativistic quantum mechanics "in the narrow sense". The subsequent discussion of quantum field theoretical corrections (admittedly without their deeper explanation) along with their excellent agreement with experimental results may perhaps provide the strongest motivation in this book to consider quantum field theories as the theoretical fundament of the Feynman rules.

Important equations and relationships are summarized in boxes to allow the reader a well-structured understanding and easy reference. Furthermore, after each section there are a short summary as well as some exercises for checking the understanding of the subject matter. The appendix contains a short compilation of important formulae and concepts.

Finally, we hope that this book helps to bridge over the gap between nonrelativistic quantum mechanics and modern quantum field theories, and explains comprehensibly the necessity for quantized fields by exposing relativistic quantum mechanics “in the narrow sense”.

Cologne, March 2010 *Armin Wachter*

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1. Relativistic Description of Spin-0 Particles

In this chapter, we deal with the relativistic description of spin-0 particles in the "narrow sense" as mentioned in the preface, i.e. on the basis of an adequate enhancement of nonrelativistic quantum mechanics. In doing so, we will adhere to the one-particle interpretation of the nonrelativistic theory to the greatest possible extent. Before we start our discussion, the principles underlying this interpretation are summarized as follows:

Theorem 1.1: Principles of nonrelativistic quantum mechanics

1) The quantum mechanical state of a physical system is described by a state vector $|\psi(t)\rangle$ in a complex unitary Hilbert space $\mathcal{H}$. In this space a positive definite scalar product $\langle\psi|\varphi\rangle$ is defined with the following properties:

- $\langle\psi|\psi\rangle \geq 0$
- $\langle\psi|\varphi\rangle = \langle\varphi|\psi\rangle^*$
- $$\begin{aligned} \langle\psi|\left(\lambda_1|\varphi_1\rangle + \lambda_2|\varphi_2\rangle\right) &= \lambda_1\langle\psi|\varphi_1\rangle + \lambda_2\langle\psi|\varphi_2\rangle \\ \left(\langle\psi_1|\lambda_1 + \langle\psi_2|\lambda_2\right)|\varphi\rangle &= \lambda_1^*\langle\psi_1|\varphi\rangle + \lambda_2^*\langle\psi_2|\varphi\rangle \ , \end{aligned}$$

  with $|\psi_{1,2}\rangle, |\varphi_{1,2}\rangle \in \mathcal{H}$, $\lambda_{1,2} \in \mathbb{C}$.

2) Physical observables are quantities that can be measured experimentally. They are described by Hermitean operators with real eigenvalues and a complete orthogonal eigenbasis. The quantum mechanical counterparts to the independent classical quantities "position" x_i and "momentum" p_i are the operators $\hat{x}_i$ and $\hat{p}_i$, for which the following commutation relations hold:

$$[\hat{x}_i, \hat{x}_j] = [\hat{p}_i, \hat{p}_j] = 0 \ , \ [\hat{x}_i, \hat{p}_j] = \mathrm{i}\hbar\delta_{ij} \ , \ i, j = 1, 2, 3 \ .$$

The Hermitean operators corresponding to the classical dynamical variables $\Omega(x_i, p_i)$ are obtained from the mapping

$$\hat{\Omega} = \Omega(x_i \to \hat{x}_i, p_i \to \hat{p}_i) \ .$$

▷

A. Wachter, Relativistic Description of Spin-0 Particles. In: A. Wachter, Relativistic Quantum Mechanics, Theoretical and Mathematical Physics, pp. 1–84 (2011)
DOI 10.1007/978-90-481-3645-2_1

However, there also exist observables without classical analogons such as the particle spin.

3) Every state vector $|\psi\rangle$ can be expanded in the orthonormal eigenbasis $\{|\omega_i\rangle\}$ of an observable $\hat{\Omega}$:

$$|\psi\rangle = \sum_i |\omega_i\rangle \langle\omega_i|\psi\rangle \ , \ \hat{\Omega}|\omega_i\rangle = \omega_i |\omega_i\rangle \ , \ \langle\omega_i|\omega_j\rangle = \delta_{ij} \ .$$

A measurement of a dynamical variable corresponding to the operator $\hat{\Omega}$ yields one of its eigenvalues ω_i with probability

$$W(\omega_i) = \frac{|\langle\omega_i|\psi\rangle|^2}{\langle\psi|\psi\rangle} \ .$$

The statistical average (expectation value) of an observable $\hat{\Omega}$, resulting from a large number of similar measurements on identical systems, is (assuming $|\psi\rangle$ is normalized such that $\langle\psi|\psi\rangle = 1$)

$$\langle\hat{\Omega}\rangle = \langle\psi|\hat{\Omega}\psi\rangle = \langle\psi|\hat{\Omega}|\psi\rangle \ .$$

4) The state vector $|\psi(t)\rangle$ satisfies the Schrödinger equation

$$\mathrm{i}\hbar\frac{\mathrm{d}|\psi(t)\rangle}{\mathrm{d}t} = \hat{H}|\psi(t)\rangle \ ,$$

where $\hat{H}$ denotes the Hermitean operator of total energy (the Hamilton operator). In the simplest case it is obtained from the Hamilton function of the corresponding classical system:

$$\hat{H} = H(x_i \to \hat{x}_i, p_i \to \hat{p}_i) \ .$$

The Hermitecity of $\hat{H}$ leads to the conservation law $\mathrm{d}\langle\psi|\psi\rangle/\mathrm{d}t = 0$.

These basic laws or axioms formulated in the Schrödinger picture can be concretized further by choosing a particular representation (or basis). In the coordinate or position representation which we will mostly use in this book, the state vector $|\psi(t)\rangle$ is represented by a wave function $\psi(\boldsymbol{x}, t)$ encompassing all space-time (and other) information of the physical system. The quantity $|\psi(\boldsymbol{x}, t)|^2$ is interpreted as a probability measure for finding the physical system at the space-time point $(\boldsymbol{x}, t)$. In this representation the position and momentum operators are given by

$$\hat{x}_i = x_i \ , \ \hat{p}_i = -\mathrm{i}\hbar\frac{\partial}{\partial x_i} \ .$$

The corresponding expressions for the scalar product and the expectation value of an observable $\hat{\Omega}$ are

$$\langle\psi|\varphi\rangle = \int \mathrm{d}^3x\psi^\dagger\varphi \ , \ \langle\psi|\hat{\Omega}|\psi\rangle = \int \mathrm{d}^3x\psi^\dagger\hat{\Omega}\psi \ .$$

From this and from the above mentioned 4th axiom follows the conservation of total probability,

$$\frac{\mathrm{d}}{\mathrm{d}t}\int \mathrm{d}^3x|\psi(\boldsymbol{x},t)|^2 = 0 \ ,$$

which is necessary for the statistical one-particle interpretation. On the basis of these principles, particularly the last relation that expresses particle number conservation – or, rather, conservation of the single considered particle – we can already now make some statements about to what extent a relativistic enhancement of the one-particle concept is at all possible.

- Due to the possibility of particle creation at interaction energies that are at least equal to the rest energy of the particle, the range of validity of the one-particle view is restricted to particle energies E, particle momenta $\boldsymbol{p}$, and electromagnetic interaction potentials A^μ, for which

  $$|E - m_0c^2| < m_0c^2 \ , \ |\boldsymbol{p}|, \left|\frac{e}{c}A^\mu\right| < m_0c \ , \ \Delta E \ll m_0c^2 \ , \ \Delta p \ll m_0c \ ,$$

  where m_0 denotes the rest mass of the particle. This is precisely the domain of the *nonrelativistic approximation.*

- Given these restrictions and Heisenberg's uncertainty relation, it follows that

  $$\Delta x \geq \frac{\hbar}{\Delta p} \gg \frac{\hbar}{m_0c} \ .$$

  This means that a relativistic particle cannot be localized more precisely than to an area whose linear extent is large compared to the particle's *Compton wave length* $\lambda_{\mathrm{c}} = \hbar/(m_0c)$.

In the subsequent discussion of the Klein-Gordon theory (as well as of the Dirac theory in the next chapter) these points will be especially taken into account and further concretized.

The main features of the Klein-Gordon theory for the relativistic description of spin-0 particles are developed in the first section of this chapter. Here we will particularly be confronted with negative energy states, which can, however, be related to *antiparticles* using the transformation of *charge conjugation.* The second section deals with the symmetry properties of the Klein-Gordon theory. In addition to continuous symmetries, discrete symmetry transformations are of particular interest as they will lead us to a deeper understanding of the negative eigensolutions. In the third section we extend and complete the one-particle picture of the Klein-Gordon theory. Introducing a *generalized scalar product*, we modify the nonrelativistic quantum mechanical framework in such a way that a consistent one-particle interpretation becomes possible. Furthermore, we discuss the range of validity of the Klein-Gordon one-particle picture and show some interpretational problems outside this range. The fourth section considers the nonrelativistic approximation of the Klein-Gordon theory. First, the nonrelativistic limit is discussed, which leads, as expected, to the laws of nonrelativistic quantum mechanics. Subsequently (higher) relativistic corrections are incorporated by expanding the Klein-Gordon equation in powers of v/c using the *Fouldy-Wouthuysen technique*. This chapter ends with the fifth section, where some simple one-particle systems are considered, particularly with a view to a consistent one-particle interpretation.

Note. To avoid misunderstandings, the terms “wave function”, “solution”, and “state” are used synonymously in the following. They all refer to the functions that solve the Klein-Gordon equation. In contrast, observable states realized in nature are termed (anti)particles. From now on, the tag “ $\hat{}$ ” for quantum mechanical operators is suppressed.

1.1 Klein-Gordon Equation

We start our discussion of the Klein-Gordon theory by writing the Klein-Gordon equation in canonical form. In doing so, we immediately come across two new phenomena, which have no reasonable interpretation within the usual quantum mechanical framework: the existence of negative energy solutions and the absence of a positive definite probability density. Following this, we bring the canonical equation into Hamilton or Schrödinger form, which will turn out to be very useful for subsequent considerations. At the end, we return to the above mentioned two phenomena and develop a physically acceptable interpretation for them using the transformation of charge conjugation.

1.1.1 Canonical and Lorentz-covariant Formulations of the Klein-Gordon Equation

In nonrelativistic quantum mechanics the starting point is the energy-momentum relation

$$E = \frac{\boldsymbol{p}^2}{2m} \;,$$

which, using the correspondence rule

$$E \longrightarrow \mathrm{i}\hbar\frac{\partial}{\partial t} \;,\; \boldsymbol{p} \longrightarrow -\mathrm{i}\hbar\boldsymbol{\nabla} \Longleftrightarrow p^\mu \longrightarrow \mathrm{i}\hbar\partial^\mu \quad \text{(four-momentum)} \;,$$

leads to the Schrödinger equation for free particles,

$$\mathrm{i}\hbar\frac{\partial\psi(\boldsymbol{x},t)}{\partial t} = -\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2\psi(\boldsymbol{x},t) \;.$$

Due to the different orders of its temporal and spatial derivatives, this equation is not Lorentz-covariant (see footnote 1 on page 352 in the Appendix A.1). This means that, passing from one inertial system to another, the equation changes its structure, thus contradicting the principle of relativity. Therefore, in order to arrive at a relativistic quantum mechanical wave equation, it is appropriate to start from the corresponding relativistic energy-momentum relation for free particles,

$$E = \sqrt{c^2 \boldsymbol{p}^2 + m_0^2 c^4} \ , \tag{1.1}$$

where m_0 denotes the rest mass of the particle. Using the above replacement, this leads to

$$\mathrm{i}\hbar \frac{\partial \phi(x)}{\partial t} = \left(-c^2 \hbar^2 \boldsymbol{\nabla}^2 + m_0^2 c^4\right)^{1/2} \phi(x) \ , \ x = (x^\mu) \ .$$

However, this equation has two grave flaws. On the one hand, due to the unsymmetrical appearance of space and time derivatives, the relativistic form invariance of this equation is not apparent. On the other hand, the operator on the right hand side is a square root whose expansion leads to a highly nonlocal theory.

Free Klein-Gordon equation. Both problems can be circumvented by starting with the quadratic form of (1.1), i.e.

$$E^2 = c^2 \boldsymbol{p}^2 + m_0^2 c^4 \Longleftrightarrow p_0^2 - \boldsymbol{p}^2 = p_\mu p^\mu = m_0^2 c^2 \ .$$

In this case, using the above correspondence rule, one obtains the *free Klein-Gordon equation in canonical form*

$$-\hbar^2 \frac{\partial^2 \phi(x)}{\partial t^2} = \left(-c^2 \hbar^2 \boldsymbol{\nabla}^2 + m_0^2 c^4\right) \phi(x) \ , \ x = (x^\mu) \ . \tag{1.2}$$

This can immediately be brought into Lorentz-covariant form,

$$\left(p_\mu p^\mu - m_0^2 c^2\right) \phi(x) = 0 \ , \tag{1.3}$$

so that, for example, the transformational behavior of the wave function ϕ is easy to anticipate when changing the reference system. This equation was suggested by Erwin Schrödinger in 1926 as a relativistic generalization of the Schrödinger equation. Later it was studied in more detail by Oskar Benjamin Klein and Walter Gordon.

First it is to be asserted that, contrary to Schrödinger's equation, the Klein-Gordon equation is a partial differential equation of second order in time. So, to uniquely specify a Klein-Gordon state, one needs two initial values, $\phi(x)$ and $\partial\phi(x)/\partial t$. Furthermore, the Klein-Gordon equation seems to be suited for the description of spin-0 particles (spinless *bosons*), since ϕ is a scalar function and does not possess any internal degrees of freedom or, put differently, the operator in (1.3) only acts on the external degrees of freedom (space-time coordinates) of ϕ.

The free solutions to (1.2) or (1.3) with definite momentum can be easily found. They are

$$\begin{aligned}\phi_{\boldsymbol{p}}^{(1)}(x) &= \mathrm{e}^{-\mathrm{i}(cp_0 t - \boldsymbol{p}\boldsymbol{x})/\hbar} \ , \ p_0 = +\sqrt{\boldsymbol{p}^2 + m_0^2c^2} > 0 \\ \phi_{\boldsymbol{p}}^{(2)}(x) &= \mathrm{e}^{+\mathrm{i}(cp_0 t - \boldsymbol{p}\boldsymbol{x})/\hbar}\end{aligned}$$

or

$$\phi_{\boldsymbol{p}}^{(r)}(x) = \mathrm{e}^{-\mathrm{i}\epsilon_r p_\mu x^\mu/\hbar} \ , \ \epsilon_r = \begin{cases} +1 \text{ for } r=1 \\ -1 \text{ for } r=2 \ . \end{cases}$$

Note that here and in the following, p_0 is always meant to be the positive square root. Obviously, the Klein-Gordon equation leads to solutions with positive energy eigenvalues $E = +cp_0$ and negative energy eigenvalues $E = -cp_0$ that are separated by the "forbidden" energy interval $]-m_0c^2; m_0c^2[$.[1] While the positive solutions can be interpreted as particle wave functions, the physical meaning of the negative solutions is not clear a priori. This makes the Klein-Gordon theory seem unattractive as a relativistic generalization of Schrödinger's theory. However, as we will see later on, negative solutions can be related to *antiparticles* that are experimentally observable so that the Klein-Gordon theory indeed provides a valuable generalization of Schrödinger's theory. Incidentally, this is why we consider $\phi_{\boldsymbol{p}}^{(2)}(x)$ to be a negative solution with momentum index $\boldsymbol{p}$, although it has the momentum eigenvalue $-\boldsymbol{p}$.

We will return to the interpretational problem of negative solutions later and investigate next some further properties of the Klein-Gordon equation.

Interaction with electromagnetic fields, gauge invariance. In the Klein-Gordon equation, the interaction of a relativistic spin-0 particle with an electromagnetic field can, as in the Schrödinger theory, be taken into account by the following operator replacement, the so-called *minimal coupling*:

$$\mathrm{i}\hbar\frac{\partial}{\partial t} \longrightarrow \mathrm{i}\hbar\frac{\partial}{\partial t} - eA^0 \ , \ \frac{\hbar}{\mathrm{i}}\boldsymbol{\nabla} \longrightarrow \frac{\hbar}{\mathrm{i}}\boldsymbol{\nabla} - \frac{e}{c}\boldsymbol{A} \Longleftrightarrow p^\mu \longrightarrow p^\mu - \frac{e}{c}A^\mu \ ,$$

where $(A^\mu) = \begin{pmatrix} A^0 \\ \boldsymbol{A} \end{pmatrix}$ denotes the electromagnetic four-potential and e the electric charge of the particle. With this, (1.2) and (1.3) become[2]

$$\left[\left(\mathrm{i}\hbar\frac{\partial}{\partial t} - eA^0\right)^2 - c^2\left(\frac{\hbar}{\mathrm{i}}\boldsymbol{\nabla} - \frac{e}{c}\boldsymbol{A}\right)^2 - m_0^2c^4\right]\phi = 0 \tag{1.4}$$

and

$$\left[\left(p_\mu - \frac{e}{c}A_\mu\right)\left(p^\mu - \frac{e}{c}A^\mu\right) - m_0^2c^2\right]\phi = 0 \ . \tag{1.5}$$

[1] In the following, the solutions whose energy eigenvalues lie above the forbidden interval (limited from below) are termed *positive solutions* and those with energy eigenvalues below the forbidden interval (limited from above) *negative solutions*.

[2] The minimal coupling is at most correct for structureless point particles which, however, have not been observed so far. Therefore, in (1.5) additional (phenomenologically based) terms of the form $\lambda F_{\mu\nu}F^{\mu\nu}\phi$ with $F^{\mu\nu} = \partial^\mu A^\nu - \partial^\nu A^\mu$ have to be, in principle, taken into consideration.

As is well-known, the Maxwell equations are invariant under local gauge transformations of the kind

$$A^0 \longrightarrow A'^0 = A^0 - \frac{1}{c}\frac{\partial \chi}{\partial t} \ , \ \boldsymbol{A} \longrightarrow \boldsymbol{A}' = \boldsymbol{A} + \boldsymbol{\nabla}\chi$$

or

$$A^\mu \longrightarrow A'^\mu = A^\mu - \partial^\mu \chi \ , \tag{1.6}$$

where $\chi = \chi(x)$ is an arbitrary real scalar function of the space-time coordinates. As in the nonrelativistic theory, this local gauge invariance can be carried over to the Klein-Gordon equation (1.4) or (1.5) by multiplying the wave function ϕ by a suitably chosen phase:

$$\phi(x) \longrightarrow \phi'(x) = e^{\mathrm{i}\Lambda(x)}\phi(x) \ . \tag{1.7}$$

In order to find the function Λ, we express (1.5) in terms of the primed quantities and calculate as follows:

$$\begin{aligned} 0 &= \left[\left(p_\mu - \frac{e}{c}A'_\mu - \frac{e}{c}\partial_\mu\chi\right)\left(p^\mu - \frac{e}{c}A'^\mu - \frac{e}{c}\partial^\mu\chi\right) - m_0^2c^2\right]\phi'\mathrm{e}^{-\mathrm{i}\Lambda} \\ &= \left[\left(p_\mu - \frac{e}{c}A'_\mu - \frac{e}{c}\partial_\mu\chi\right)\mathrm{e}^{-\mathrm{i}\Lambda}\left(p^\mu - \frac{e}{c}A'^\mu - \frac{e}{c}\partial^\mu\chi + \hbar\partial^\mu\Lambda\right)\right. \\ &\quad \left. - \, m_0^2c^2\mathrm{e}^{-\mathrm{i}\Lambda}\right]\phi' \\ &= \mathrm{e}^{-\mathrm{i}\Lambda}\left[\left(p_\mu - \frac{e}{c}A'_\mu - \frac{e}{c}\partial_\mu\chi + \hbar\partial_\mu\Lambda\right)\left(p^\mu - \frac{e}{c}A'^\mu - \frac{e}{c}\partial^\mu\chi + \hbar\partial^\mu\Lambda\right)\right. \\ &\quad \left. - \, m_0^2c^2\right]\phi' \ . \end{aligned} \tag{1.8}$$

Choosing

$$\Lambda(x) = \frac{e}{\hbar c}\chi(x) \ , \tag{1.9}$$

(1.8) becomes

$$\left[\left(p_\mu - \frac{e}{c}A'_\mu\right)\left(p^\mu - \frac{e}{c}A'^\mu\right) - m_0^2c^2\right]\phi' = 0 \ ,$$

which is formally identical to the Klein-Gordon equation (1.5). Since physical observables are represented by bilinear forms of the kind $\langle \phi^* | \ldots | \phi \rangle$, a common equal phase factor does not play any role. Therefore, the Klein-Gordon equation with minimal coupling is invariant under local gauge transformations of the electromagnetic field.[3]

[3] Remarkably, the transformation (1.7) along with (1.9) is the same as the transformation that leads to local gauge invariance in the nonrelativistic theory.

Continuity equation. Multiplying (1.4) or (1.5) by ϕ^* from the left and subsequently subtracting the complex conjugate, one obtains a continuity equation of the form

$$\frac{\partial \rho(x)}{\partial t} + \boldsymbol{\nabla} \boldsymbol{j}(x) = 0 \ , \tag{1.10}$$

with

$$\begin{aligned} \rho(x) &= \frac{\mathrm{i}\hbar}{2m_0c^2}\left[\phi^*\frac{\partial \phi}{\partial t} - \left(\frac{\partial \phi^*}{\partial t}\right)\phi\right] - \frac{e}{m_0c^2}A^0\phi^*\phi \\ \boldsymbol{j}(x) &= -\frac{\mathrm{i}\hbar}{2m_0}\left[\phi^*\boldsymbol{\nabla}\phi - (\boldsymbol{\nabla}\phi^*)\phi\right] - \frac{e}{m_0c}\boldsymbol{A}\phi^*\phi \end{aligned}$$

or, in Lorentz-covariant notation,

$$\partial_\mu j^\mu(x) = 0 \ , \ j^\mu = \frac{\mathrm{i}\hbar}{2m_0}\left(\phi^*\partial^\mu\phi - \phi\partial^\mu\phi^*\right) - \frac{e}{m_0c}A^\mu\phi^*\phi \ , \ (j^\mu) = \begin{pmatrix} c\rho \\ \boldsymbol{j} \end{pmatrix} .$$

Note that an overall factor was introduced in ρ and $\boldsymbol{j}$ due to analogy with nonrelativistic quantum mechanics. As usual, spatial integration of (1.10) yields the conservation law

$$Q = \int \mathrm{d}^3x \rho(x) = \text{const} \ .$$

Obviously, $\rho(x)$ is not positive definite since, at a given time t, ϕ and $\partial\phi/\partial t$ can take on arbitrary values. Therefore, ρ and $\boldsymbol{j}$ cannot be interpreted as probability quantities. This problem, in conjunction with the existence of negative solutions, was the reason that the Klein-Gordon equation was initially rejected and that attempts were made to find a relativistic wave equation of first order in time and with a positive definite probability density. This equation was indeed found by Dirac. However, as we see in Chapter 2, the Dirac equation also yields solutions with negative energy eigenvalues.

To summarize:

Theorem 1.2: Klein-Gordon equation in canonical and Lorentz-covariant forms

The Klein-Gordon equation is the relativistic generalization of Schrödinger's equation for spin-0 particles. For a minimal coupled electromagnetic field, it is

$$\left[\left(\mathrm{i}\hbar\frac{\partial}{\partial t} - eA^0\right)^2 - c^2\left(\frac{\hbar}{\mathrm{i}}\boldsymbol{\nabla} - \frac{e}{c}\boldsymbol{A}\right)^2 - m_0^2c^4\right]\phi(x) = 0 \tag{1.11}$$

or, in manifestly covariant notation,

$$\left[\left(p_\mu - \frac{e}{c}A_\mu\right)\left(p^\mu - \frac{e}{c}A^\mu\right) - m_0^2c^2\right]\phi(x) = 0 \ , \tag{1.12}$$

▷

where m_0 is the rest mass and e the electric charge of the particle. These equations are invariant under local gauge transformations of the electromagnetic field. From the Klein-Gordon equation follows the continuity equation

$$\partial_\mu j^\mu = 0 \ , \ (j^\mu) = \begin{pmatrix} c\rho \\ \boldsymbol{j} \end{pmatrix} \ ,$$

with

$$\left.\begin{aligned} \rho(x) &= \frac{\mathrm{i}\hbar}{2m_0c^2}\left[\phi^*\frac{\partial\phi}{\partial t} - \left(\frac{\partial\phi^*}{\partial t}\right)\phi\right] - \frac{e}{m_0c^2}A^0\phi^*\phi \\ \boldsymbol{j}(x) &= -\frac{\mathrm{i}\hbar}{2m_0}\left[\phi^*\boldsymbol{\nabla}\phi - (\boldsymbol{\nabla}\phi^*)\phi\right] - \frac{e}{m_0c}\boldsymbol{A}\phi^*\phi \ , \end{aligned}\right\} \tag{1.13}$$

as well as the conservation law

$$Q = \int \mathrm{d}^3x\rho(x) = \text{const} \ .$$

The solutions to the free Klein-Gordon equation ($A^\mu = 0$) are

$$\phi_{\boldsymbol{p}}^{(r)}(x) = \frac{1}{(2\pi\hbar)^{3/2}}\sqrt{\frac{m_0c}{p_0}}\mathrm{e}^{-\mathrm{i}\epsilon_r p_\mu x^\mu/\hbar} \ , \ p_0 = +\sqrt{\boldsymbol{p}^2 + m_0^2c^2} \ ,$$

with momentum eigenvalue $+\boldsymbol{p}$ (for $r = 1$) or $-\boldsymbol{p}$ (for $r = 2$). These solutions are normalized such that

$$\frac{\mathrm{i}\hbar}{2m_0c^2}\int \mathrm{d}^3x\left[\phi_{\boldsymbol{p}}^{(r)*}\frac{\partial\phi_{\boldsymbol{p}'}^{(r')}}{\partial t} - \left(\frac{\partial\phi_{\boldsymbol{p}}^{(r)*}}{\partial t}\right)\phi_{\boldsymbol{p}'}^{(r')}\right] = \epsilon_r\delta_{rr'}\delta(\boldsymbol{p} - \boldsymbol{p}') \ .$$

1.1.2 Hamilton Formulation of the Klein-Gordon Equation

The Klein-Gordon equation from Theorem 1.2 is a differential equation of second order in time. For our subsequent discussion, it is useful to convert it into a system of coupled differential equations of first temporal order. In this way, it acquires a Schrödinger-like form, in which a Hamilton operator can be identified just as in the nonrelativistic theory. Introducing two new fields via

$$\phi = \varphi + \chi \ , \ \left(\mathrm{i}\hbar\frac{\partial}{\partial t} - eA^0\right)\phi = m_0c^2(\varphi - \chi) \tag{1.14}$$

$$\Longrightarrow \left\{\begin{aligned} \varphi &= \frac{1}{2m_0c^2}\left(m_0c^2 + \mathrm{i}\hbar\frac{\partial}{\partial t} - eA^0\right)\phi \\ \chi &= \frac{1}{2m_0c^2}\left(m_0c^2 - \mathrm{i}\hbar\frac{\partial}{\partial t} + eA^0\right)\phi \ , \end{aligned}\right. \tag{1.15}$$

(1.11) can be rewritten as

$$\begin{aligned}\left(\mathrm{i}\hbar\frac{\partial}{\partial t} - eA^0\right)(\varphi + \chi) &= m_0c^2(\varphi - \chi)\\ \left(\mathrm{i}\hbar\frac{\partial}{\partial t} - eA^0\right)(\varphi - \chi) &= \left[\frac{1}{m_0}\left(\boldsymbol{p} - \frac{e}{c}\boldsymbol{A}\right)^2 + m_0c^2\right](\varphi + \chi)\ .\end{aligned}$$

Addition and subtraction of these two equations lead to the system of coupled differential equations of first order in time,

$$\begin{aligned}\mathrm{i}\hbar\frac{\partial\varphi}{\partial t} &= \frac{1}{2m_0}\left(\boldsymbol{p} - \frac{e}{c}\boldsymbol{A}\right)^2(\varphi + \chi) + (m_0c^2 + eA^0)\varphi\\ \mathrm{i}\hbar\frac{\partial\chi}{\partial t} &= -\frac{1}{2m_0}\left(\boldsymbol{p} - \frac{e}{c}\boldsymbol{A}\right)^2(\varphi + \chi) - (m_0c^2 - eA^0)\chi\ ,\end{aligned}$$

which is equivalent to (1.11). Finally pooling φ and χ into

$$\psi = \begin{pmatrix}\varphi\\ \chi\end{pmatrix}$$

leads to the *Klein-Gordon equation in Hamilton form*

$$\mathrm{i}\hbar\frac{\partial\psi}{\partial t} = H\psi\ ,\ H = \frac{\tau_3 + \mathrm{i}\tau_2}{2m_0}\left(\boldsymbol{p} - \frac{e}{c}\boldsymbol{A}\right)^2 + \tau_3 m_0c^2 + eA^0\ .$$

Here τ_i denote the *Pauli matrices*

$$\tau_1 = \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\ ,\ \tau_2 = \begin{pmatrix}0 & -\mathrm{i}\\ \mathrm{i} & 0\end{pmatrix}\ ,\ \tau_3 = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\ ,$$

which satisfy the following algebra:

$$\tau_i\tau_j = i\epsilon_{ijk}\tau_k + \delta_{ij}\ ,\ [\tau_i,\tau_j] = 2i\epsilon_{ijk}\tau_k\ ,\ \{\tau_i,\tau_j\} = 2\delta_{ij}\ .$$

The solutions to the free Klein-Gordon equation

$$\mathrm{i}\hbar\frac{\partial\psi}{\partial t} = H^{(0)}\psi\ ,\ H^{(0)} = \frac{(\tau_3 + \mathrm{i}\tau_2)\boldsymbol{p}^2}{2m_0} + \tau_3 m_0c^2 \tag{1.16}$$

are given by (see Exercise 1)

$$\begin{aligned}\psi_{\boldsymbol{p}}^{(1)}(x) &= \begin{pmatrix}m_0c + p_0\\ m_0c - p_0\end{pmatrix}\mathrm{e}^{-\mathrm{i}p_\mu x^\mu/\hbar}\\ \psi_{\boldsymbol{p}}^{(2)}(x) &= \begin{pmatrix}m_0c - p_0\\ m_0c + p_0\end{pmatrix}\mathrm{e}^{+\mathrm{i}p_\mu x^\mu/\hbar}\ .\end{aligned}$$

To calculate ρ and $\boldsymbol{j}$ in the Hamilton formulation, we insert (1.14) and (1.15) into (1.13) and obtain

$$\begin{aligned}\rho(x) &= \psi^\dagger(x)\tau_3\psi(x) = \varphi^*\varphi - \chi^*\chi\\ \boldsymbol{j}(x) &= -\frac{\mathrm{i}\hbar}{2m_0}\left[\psi^\dagger\tau_3(\tau_3 + \mathrm{i}\tau_2)\boldsymbol{\nabla}\psi - (\boldsymbol{\nabla}\psi^\dagger)\tau_3(\tau_3 + \mathrm{i}\tau_2)\psi\right]\\ &\quad -\frac{e}{m_0c}\boldsymbol{A}\psi^\dagger\tau_3(\tau_3 + \mathrm{i}\tau_2)\psi\ .\end{aligned}$$

Overall, we arrive at the following theorem equivalent to Theorem 1.2:

Theorem 1.3: Klein-Gordon equation in Hamilton form

With the replacements

$$\phi = \varphi + \chi \ , \ \left(\mathrm{i}\hbar\frac{\partial}{\partial t} - eA^0\right)\phi = m_0c^2(\varphi - \chi) \ , \ \psi = \begin{pmatrix}\varphi \\ \chi\end{pmatrix}$$

in (1.11), the Klein-Gordon equation in Hamilton form follows as

$$\mathrm{i}\hbar\frac{\partial\psi}{\partial t} = H\psi \ , \ H = \frac{\tau_3 + \mathrm{i}\tau_2}{2m_0}\left(\boldsymbol{p} - \frac{e}{c}\boldsymbol{A}\right)^2 + \tau_3 m_0 c^2 + eA^0 \ , \tag{1.17}$$

where τ_i denote the Pauli matrices. The corresponding expressions for ρ and $\boldsymbol{j}$ are

$$\begin{aligned}
\rho(x) &= \psi^\dagger(x)\tau_3\psi(x) = \varphi^*\varphi - \chi^*\chi \\
\boldsymbol{j}(x) &= -\frac{\mathrm{i}\hbar}{2m_0}\left[\psi^\dagger\tau_3(\tau_3 + \mathrm{i}\tau_2)\boldsymbol{\nabla}\psi - (\boldsymbol{\nabla}\psi^\dagger)\tau_3(\tau_3 + \mathrm{i}\tau_2)\psi\right] \\
&\quad -\frac{e}{m_0c}\boldsymbol{A}\psi^\dagger\tau_3(\tau_3 + \mathrm{i}\tau_2)\psi \\
Q &= \int \mathrm{d}^3x\rho(x) = \int \mathrm{d}^3x\psi^\dagger(x)\tau_3\psi(x) \ .
\end{aligned}$$

In the Hamilton formulation, the solutions to the free Klein-Gordon equations are

$$\left.\begin{aligned}
\psi_{\boldsymbol{p}}^{(r)}(x) &= \frac{1}{(2\pi\hbar)^{3/2}}\Psi^{(r)}(\boldsymbol{p})\mathrm{e}^{-\mathrm{i}\epsilon_r p_\mu x^\mu/\hbar} \\
\Psi^{(r)}(\boldsymbol{p}) &= \frac{1}{2\sqrt{m_0cp_0}}\begin{pmatrix} m_0c + \epsilon_r p_0 \\ m_0c - \epsilon_r p_0\end{pmatrix} \ ,
\end{aligned}\right\} \tag{1.18}$$

with momentum eigenvalue $+\boldsymbol{p}$ (for $r = 1$) or $-\boldsymbol{p}$ (for $r = 2$). These solutions are normalized such that

$$\int \mathrm{d}^3x\psi_{\boldsymbol{p}}^{(r)\dagger}(x)\tau_3\psi_{\boldsymbol{p}'}^{(r')}(x) = \epsilon_r\delta_{rr'}\delta(\boldsymbol{p} - \boldsymbol{p}')$$

$$\Psi^{(r)\dagger}(\boldsymbol{p})\tau_3\Psi^{(r')}(\boldsymbol{p}) = \epsilon_r\delta_{rr'} \ , \ \Psi^{(r)}(\boldsymbol{p}) = \Psi^{(r)}(-\boldsymbol{p}) \ . \tag{1.19}$$

It is important to note that in (1.17) the Hamilton operator H is not Hermitean (since $\mathrm{i}\tau_2$ is not Hermitean). From this it immediately becomes apparent, why it is impossible to find a positive definite probability density (including total probability conservation): using the nonrelativistic scalar product

$$\langle\psi|\phi\rangle = \int \mathrm{d}^3x\psi^\dagger\phi \ , \ \langle\psi|\mathcal{O}|\phi\rangle = \int \mathrm{d}^3x\psi^\dagger\mathcal{O}\phi \tag{1.20}$$

and the adjunction relation

$$\langle\psi|\mathcal{O}|\phi\rangle = \left\langle\phi|\mathcal{O}^\dagger|\psi\right\rangle^* \qquad (\mathcal{O}\text{ linear operator}) \ , \tag{1.21}$$

we have

$$\mathrm{i}\hbar\frac{\partial\psi}{\partial t} = H\psi \Longrightarrow \mathrm{i}\hbar\psi^\dagger\frac{\partial\psi}{\partial t} = \psi^\dagger H\psi\ ,\ -\mathrm{i}\hbar\frac{\partial\psi^\dagger}{\partial t}\psi = (H\psi)^\dagger\psi = (\psi^\dagger H\psi)^*$$

$$\Longrightarrow \mathrm{i}\hbar\frac{\partial}{\partial t}\langle\psi|\,\psi\rangle = \langle\psi|\,H\,|\psi\rangle - \langle\psi|\,H\,|\psi\rangle^* = \left\langle\psi\right|H - H^\dagger\left|\psi\right\rangle \neq 0\ .$$

Furthermore, the non-Hermitecity of H is the reason that its eigenstates are generally not orthogonal with respect to (1.20).

Another important consequence of the non-Hermitecity of H is that $\mathrm{e}^{\mathrm{i}H}$ is not unitary. This is one indication that in the Klein-Gordon theory the usage of the scalar product (1.20) seems to be unsuitable as it leads to different results in different pictures (for example, the Schrödinger picture used here, or the Heisenberg picture). We will tackle this problem in Subsection 1.3.1.

1.1.3 Interpretation of Negative Solutions, Antiparticles

So far, we have written down the Klein-Gordon equation in canonical, Lorentz-covariant, and Hamilton forms and looked at some of its formal properties. Now we turn to the negative Klein-Gordon solutions which we have so far ignored. Our aim is to find a physically meaningful interpretation for them as well as for the quantities Q, ρ, and $\boldsymbol{j}$.

Charge conjugation $\boldsymbol{C}$. We again consider the canonical Klein-Gordon equation

$$\left[\left(\mathrm{i}\hbar\frac{\partial}{\partial t} - eA^0\right)^2 - c^2\left(\boldsymbol{p} - \frac{e}{c}\boldsymbol{A}\right)^2 - m_0^2c^4\right]\phi^{(-)}(x) = 0\ , \tag{1.22}$$

where $\phi^{(-)}$ denotes a solution with negative energy. Transforming this equation by taking its complex conjugate, one obtains the mathematically equivalent relation

$$\left[\left(\mathrm{i}\hbar\frac{\partial}{\partial t} + eA^0\right)^2 - c^2\left(\boldsymbol{p} + \frac{e}{c}\boldsymbol{A}\right)^2 - m_0^2c^4\right]\phi_C^{(-)}(x) = 0\ , \tag{1.23}$$

with

$$\phi_C^{(-)}(x) = \phi^{(-)*}(x)\ .$$

The consequences of this become even clearer if we start from the eigenvalue equation of a negative eigenstate $\Psi^{(-)}$ in Hamilton form,

$$\left[\frac{\tau_3 + \mathrm{i}\tau_2}{2m_0}\left(\boldsymbol{p} - \frac{e}{c}\boldsymbol{A}\right)^2 + \tau_3 m_0c^2 + eA^0\right]\Psi^{(-)}(\boldsymbol{x}) = -|E|\Psi^{(-)}(\boldsymbol{x})\ , \tag{1.24}$$

and apply complex conjugation to it. This yields

$$\left[\frac{\tau_3 + \mathrm{i}\tau_2}{2m_0}\left(\boldsymbol{p} + \frac{e}{c}\boldsymbol{A}\right)^2 + \tau_3 m_0c^2 - eA^0\right]\Psi_C^{(-)}(\boldsymbol{x}) = +|E|\Psi_C^{(-)}(\boldsymbol{x})\ , \tag{1.25}$$

with

$$\Psi_C^{(-)}(x) = \tau_1 \Psi^{(-)*}(x) \ .$$

All in all, if $\phi^{(-)}$ or $\psi^{(-)}$ describes a negative Klein-Gordon state with charge $+e$ within the potential A^μ, then $\phi_C^{(-)} = \phi^{(-)*}$ or $\psi_C^{(-)} = \tau_1 \psi^{(-)*}$ describes a positive Klein-Gordon state with charge $-e$ within the same potential A^μ. Correspondingly, the above transformation is called *charge conjugation*. Obviously, it is a reciprocal transformation since its twofold application leads back to the original equation. Furthermore, it is antilinear [4], since, going from (1.22) to (1.23), the relative sign between the differential and potential terms is changed. Therefore, charge conjugation opens us a way to a physical interpretation of negative Klein-Gordon solutions whose charge conjugates are to be regarded as the quantum mechanical wave functions of antiparticles with charge $-e$.

As regards the free Klein-Gordon solutions, charge conjugation yields

$$\phi_{\boldsymbol{p},C}^{(1,2)}(x) = \phi_{\boldsymbol{p}}^{(2,1)}(x) \ , \ \psi_{\boldsymbol{p},C}^{(1,2)}(x) = \psi_{\boldsymbol{p}}^{(2,1)}(x) \ .$$

In this case the original as well as the charge conjugated wave functions are solutions to the same equation, because the distinction between free states with different charges is not possible.

Charge density, charge current density. We are now in a position to give the quantities Q, ρ, and $\boldsymbol{j}$ physically meaningful interpretations. As we have seen above, the quantity

$$\rho = \psi^\dagger \tau_3 \psi = \varphi^* \varphi - \chi^* \chi \ , \ \int \mathrm{d}^3 x \rho(x) = Q = \mathrm{const}$$

cannot generally be taken as a probability density, since it is not positive definite. However, if we restrict ourselves to the validity range of the one-particle interpretation (to be more accurately defined later), i.e. to the nonrelativistic approximation mentioned at the beginning of this chapter, ρ becomes positive definite for positive Klein-Gordon solutions, $|\varphi| \gg |\chi|$, and negative for negative solutions, $|\varphi| \ll |\chi|$ (see Subsection 1.4.1). Since positive solutions belong to particles with charge $+e$ and the charge conjugates of negative solutions belong to antiparticles with charge $-e$, we can interpret the expressions $\rho^{(\pm)}$ (built by $\psi^{(\pm)}$) as *electric charge density* and $\boldsymbol{j}^{(\pm)}$ as *electric charge current density* of a particle or an antiparticle. Consequently, $Q^{(\pm)} = \pm 1$ is the (conserved) total charge of the particle or antiparticle (*charge interpretation*).[5]

[4] An operator $\mathcal{O}$ is called antilinear if $\mathcal{O}(\alpha_1 \psi_1 + \alpha_2 \psi_2) = \alpha_1^* \mathcal{O} \psi_1 + \alpha_2^* \mathcal{O} \psi_2$.

[5] This interpretation can also be maintained outside the validity range of the one-particle picture. In this case Q denotes the conserved total charge of all particles and antiparticles. Consequently, the charge density ρ may take on different signs at different space-time points.

Theorem 1.4: Charge conjugation C and charge interpretation in the Klein-Gordon theory

- In the Klein-Gordon theory the charge conjugation C is defined by the transformation

$$\phi(x) \longrightarrow \phi_C(x) = \phi^*(x) \quad \text{(canonical form)}$$

$$\psi(x) \longrightarrow \psi_C(x) = \tau_1\psi^*(x) \text{ (Hamilton form).}$$

  It turns a positive [negative] Klein-Gordon solution of charge $+e$ [$-e$] into a negative [positive] Klein-Gordon solution of charge $-e$ [$+e$].

- A positive Klein-Gordon solution $\phi^{(+)}$ or $\psi^{(+)}$ represents a physical spin-0 particle of charge $+e$ within the potential A^μ, while the charge conjugate of the negative solution $\phi_C^{(-)}$ or $\psi_C^{(-)}$ (and not the original negative solution) describes the physical antiparticle with opposite charge $-e$ within the same potential A^μ.

- The quantities Q, ρ, and $\boldsymbol{j}$ that are composed of $\phi^{(+)}$ or $\psi^{(+)}$ [$\phi^{(-)}$ or $\psi^{(-)}$] can be interpreted as the electric charge, charge density, and charge current density of the physical particle [antiparticle] (charge interpretation).

While the wave function of an antiparticle is described by the charge conjugated negative solution, one obtains its charge quantities Q, ρ, and $\boldsymbol{j}$ using the original negative solutions. In Section 1.3, we extend this principle to the definition of picture-independent scalar products and expectation values.

Now it becomes clear why we have assigned the negative free Klein-Gordon solution $\phi_{\boldsymbol{p}}^{(2)}$ [$\psi_{\boldsymbol{p}}^{(2)}$] the index $\boldsymbol{p}$, although it possesses the momentum eigenvalue $-\boldsymbol{p}$. This is because this solution should be associated with the corresponding antiparticle (with opposite momentum and energy eigenvalue).

That the statements of Theorem 1.4 do in fact agree with nature is confirmed, on the one hand, by the experimental fact that, for each known spin-0 particle, a corresponding antiparticle has been found. On the other hand, as we see in Chapter 3, they are in accordance with experimentally verifiable predictions from scattering theory.

Overall, we see that the relativistic generalization of Schrödinger's theory to the Klein-Gordon theory leads to a new degree of freedom, the electric charge, whereas the nonrelativistic theory describes states with only one charge sign.[6] In this context it is also important to note that in our considerations we could have equally started with the Klein-Gordon equation for states of charge $-e$, since the sign of the charge does not play a decisive role at any stage. Consequently, particles would carry the charge $-e$ described

[6] This is a characteristic of all relativistic enhancements.

by positive solutions, and antiparticles would have the charge $+e$ described by the charge conjugated negative solutions.

Interpretation of the negative solutions. Although we were able to give the charge conjugated negative Klein-Gordon solutions a physically meaningful interpretation, there are still two serious points open, namely:

- the physical implications stemming from the mere existence of negative solutions and
- the physical interpretation of the negative solutions.

In our previous considerations the existence of solutions with negative energy leads to problems and physical nonsense. Think, for example, of a pion atom consisting of a positively charged nucleus and a circuiting negatively charged pion (spin-0 particle). The corresponding energy spectrum can be calculated, for example, by incorporating the Coulomb potential into the Klein-Gordon equation (see Subsection 1.5.4). It is depicted qualitatively in Figure 1.1.

The bound states directly below the positive energy continuum with $E < m_0c^2$ generally agree with experimental results. So there is no doubt that these are the true bound states of the pion atom. On the other hand, the existence of the negative energy continuum implies that a ground state pion could fall deeper and deeper through continuous radiation transitions.

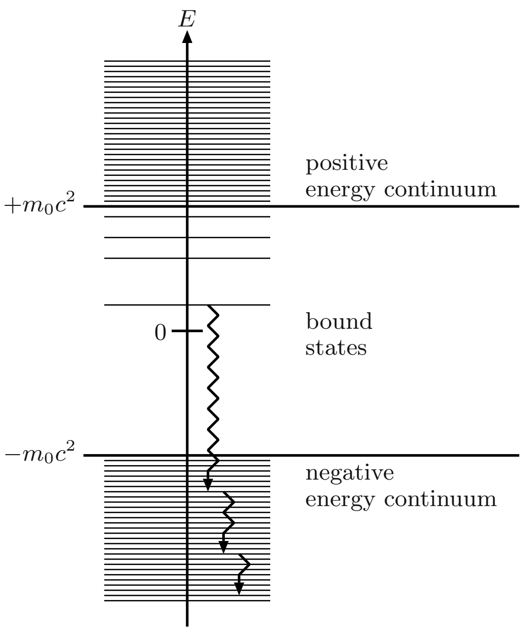

Fig. 1.1. Qualitative energy spectrum of a pion atom. Due to the existence of negative energy states, the pion could fall deeper and deeper through continuous radiation transitions.

Accordingly, the atom would be unstable and a *radiation catastrophe* would occur due to the continuous emission of light.[7] Nevertheless, it is clear that none of these effects are observed; our world could not exist if this decay was present.

As we see later, the same problem exists in the Dirac theory for describing spin-1/2 particles. But there Dirac introduced a trick known as the *hole theory* in order to avoid the radiation catastrophe. According to this model, the vacuum is regarded as a "sea" completely occupied by spin-1/2 particles with negative energies, which, due to Pauli's exclusion principle, cannot be filled by any further particles. Apart from the fact that the radiation catastrophe is now avoided, the negative states acquire a direct physical meaning with physical consequences, for example, the creation and annihilation of particle-antiparticle pairs or the *vacuum polarization*.

It is clear that the hole theory cannot be transferred to the spin-0 case in hand, since the Pauli principle does not apply here. However, even if the hole theory could be applied here in some way, it is to be kept in mind that, in any case, it would mean turning away from the one-particle concept toward a many-particle theory (with infinitely many degrees of freedom). Therefore, within the framework of the targeted one-particle interpretation, we have to leave the physical interpretation of the negative solutions open.

Résumé. All in all, it can be ascertained that using the concepts of charge conjugation and charge interpretation, we can give the positive and the charge conjugated negative energy solutions as well as Q, ρ, and $\boldsymbol{j}$ physically meaningful interpretations as particle, antiparticle, charge, charge density, and charge current density. However, with a view to a consistent one-particle interpretation in the usual nonrelativistic quantum mechanical sense, three points are still open:

[1] The one-particle interpretation requires that positive and negative solutions can be completely decoupled from one another, i.e. that each charged Klein-Gordon state can be represented by a superposition of pure negative or pure positive solutions. However, in general, a Klein-Gordon state is composed of the complete system of positive and negative solutions. We therefore have to clarify under which conditions or within which limits a complete decoupling of positive and negative solutions is possible. Such a splitting leads simultaneously to a positive or negative definite charge density so that a quantum mechanical statistical interpretation becomes possible.

[2] A complete decoupling of positive and negative solutions also implies that not all relativistic operators are applicable with respect to the one-particle concept since they generally mix positive and negative solutions. Hence,

[7] Strictly speaking, the pion atom is unstable due to other effects. However, these effects happen much more slowly than the atom's life time as predicted according to the radiation transitions into negative energy levels.