# Chapter 3

# The Klein-Gordon Equation

## 3.1 Physical Problems of the Klein-Gordon Equation

The Klein-Gordon equation (2.66) fulfills the laws of special relativity, but contains two fundamental problems, which have to be taken care of for the equation to be physically meaningful.

The first problem becomes obvious when considering the solutions of the different equations. Using the ansatz

$$\begin{aligned} \psi(x) &= a\ e^{i(\vec{k}\cdot\vec{r}\ -\ \omega t)} \\ &= a\ e^{-ik_\mu x^\mu} \end{aligned} \tag{3.1}$$

with

$$k_\mu = \begin{pmatrix} \frac{w}{c} \\ -\vec{k} \end{pmatrix} . \tag{3.2}$$

One obtains from (2.71)

$$a \left[ -k_\mu k^\mu \ + \ \left(\frac{mc}{\hbar}\right)^2 \right] = 0 \tag{3.3}$$

or

$$k^2 = k_\mu k^\mu = \left(\frac{mc}{\hbar}\right)^2 \tag{3.4}$$

from which follows

$$
\begin{aligned}
(k^0)^2 &= \vec{k}^{\,2} + \left(\frac{mc}{\hbar}\right)^2 \\
k^0 &= \pm \sqrt{\vec{k}^{\,2} + \left(\frac{mc}{\hbar}\right)^2}
\end{aligned}
\tag{3.5}
$$

This means that the Klein-Gordon equation allows negative energies as solution. Formally, one can see that from the square of Eq. (2.60) the information about the sign is lost. However, when starting from Eq. (2.71) all solutions have to be considered, and there is the **problem of the physical interpretation of negative energies**.

The second problem with the Klein-Gordon equation is less obvious. It occurs when interpreting the function $\psi(x)$ as probability amplitude. Interpretation of $\psi(x)$ as probability amplitude is only possible if there exists a probability density $\rho(x)$ and a current $\vec{j}\,(x)$ that fulfill a continuity equation

$$
\frac{\partial}{\partial t}\,\rho \,+ \vec{\nabla} \cdot \vec{j} \;=\; 0 \;, \tag{3.6}
$$

which guarantees that no "probability" is lost.

Since we deal with a covariant equation, we define

$$
\begin{aligned}
j^0(x) &:= c\rho(x) \\
j^\mu(x) &:= \begin{pmatrix} j^0(x) \\ \vec{j}\,(x) \end{pmatrix}
\end{aligned}
\tag{3.7}
$$

and obtain the covariant form

$$
\frac{\partial}{\partial x^\mu}\, j^\mu \;=\; \partial_\mu\, j^\mu \;=\; 0 \;. \tag{3.8}
$$

Eqs. (3.6) and (3.7) correspond in form and content the charge conservation in electrodynamics.

Non-relativistically one has

$$
\begin{aligned}
\rho_{NR} &= \psi^*\,\psi \\
\vec{j}_{NR} &= \frac{\hbar}{(2mi)}\,[\psi^* \;\overleftrightarrow{\nabla}\; \psi]
\end{aligned}
\tag{3.9}
$$

and thus one expects in the relativistic case also bilinear expressions in $\psi$ for $\rho$ and $\vec{j}$. If one defines a density $\rho$ according to (3.9) with the solution (3.1), it is easy to show that this density does not fulfill a continuity equation. This has to be expected since $j^\mu$ has to be a four-vector so that (3.7) is valid in all Lorentz systems. Thus, it is obvious to generalize (3.9) to

$$j^\mu := \frac{i\hbar}{2m} \psi^* \overleftrightarrow{\partial^\mu} \psi \tag{3.10}$$

where

$$A^* \overleftrightarrow{\partial^\mu} B := A^* (\partial^\mu B) - (\partial^\mu A^*) B . \tag{3.11}$$

Consider

$$\begin{aligned} \partial_\mu j^\mu &= \frac{i\hbar}{2m} \partial_\mu \left( \psi^* \overleftrightarrow{\partial^\mu} \psi \right) \\ &= \frac{i\hbar}{2m} \left[ (\partial_\mu \psi^*)(\partial^\mu \psi) + \psi^*(\partial_\mu \partial^\mu \psi) - (\partial_\mu \partial^\mu \psi^*)\psi - (\partial^\mu \psi^*)(\partial_\mu \psi) \right] \\ &= \frac{i\hbar}{2m} \left[ \psi^*(\Box\psi) - (\Box\psi^*)\psi \right] \end{aligned} \tag{3.12}$$

If $\psi$ fulfills the Klein-Gordon equation, the right-hand side of (3.12) vanishes, and the continuity equation (3.7) holds. However, the four-vector defined in (3.10) contains the second problem:

$$\begin{aligned} \rho &= \frac{1}{c} j^0 \\ &= \frac{i\hbar}{2mc} \psi^* \overleftrightarrow{\partial^0} \psi \\ &= \frac{i\hbar}{2mc^2} \left[ \psi^* \frac{\partial}{\partial t} \psi - \frac{\partial \psi^*}{\partial t} \psi \right] \end{aligned} \tag{3.13}$$

can be positive or negative, depending on the values of $\psi$ and $\frac{\partial\psi}{\partial t}$.

Since the Klein-Gordon equation denotes a partial differential equation (2nd order) of hyperbolic type, one has the option to arbitrarily choose the functions

$$\psi(\vec{x}, t = 0) \quad \text{and} \quad \frac{\partial}{\partial t} \psi(\vec{x}, t = 0) \tag{3.14}$$

at the starting time ($t = 0$), and thus obtain, e.g., negative values for $\rho(\vec{x}, t = 0)$. An interpretation of $\rho$ as probability density would mean that the theory allows negative probabilities. This is the problem of the **indefinite probability density**.

The solution of both problems has an interesting historical development, which can briefly be summarized as follows:

- 1928: Dirac "invents" the Dirac equation. The probability density is positive; however, negative energies are allowed (Proc. Roy. Soc. **A117**, 610-628).
- 1930: Dirac solves the problem of negative energies via the "hole" theory. Antiparticles are related to negative energy eigenstates (Proc. Cambridge Phil. Soc. **26**, 376-381).
- 1934: Pauli and Weisskopf present a new interpretation of the Klein-Gordon equation: as field equation for a charged spin-0 field. $\rho$ represents the charge density. Instead through $k^0$, the energy is given via $\frac{1}{2} \int d^3r \, [\mid \vec{\nabla}\psi \mid^2 + m^2 \mid \psi \mid^2]$ and thus per definition positive (Helv. Phys. Acta **7**, 709-734).
- 1934: The Dirac equation acquires a field-theoretic interpretation: It does no longer determine a probability amplitude, rather the field operator for a spin -$\frac{1}{2}$ field.

In the following, we concentrate on the first two topics, the last two are subjects of quantum field theory.

## 3.2 Nonrelativistic Limit of the Klein-Gordon Equation

We start from the form of the Klein-Gordon equation

$$\left(\Box + \frac{m^2c^2}{\hbar^2}\right)\psi = 0 \tag{3.15}$$

To study the nonrelativistic limit, we make the ansatz

$$\psi(\mathbf{x},t) = \varphi(\mathbf{x},t)\exp(-\frac{i}{\hbar}mc^2t), \tag{3.16}$$

i.e. we split off a term containing the rest mass. In the nonrelativistic limit, the difference of total energy $E$ and rest mass $mc^2$ is supposed to be small. Thus define

$$E' = E - mc^2 \tag{3.17}$$

with $E' \ll mc^2$. Thus,

$$|i\hbar\frac{\partial\varphi}{\partial t}| \approx E'\varphi \ll mc^2\varphi \tag{3.18}$$

Now consider

$$\begin{aligned}
\frac{\partial\psi}{\partial t} &= \left(\frac{\partial\varphi}{\partial t} - i\frac{mc^2}{\hbar}\varphi\right)\exp(-\frac{i}{\hbar}mc^2t) \approx -i\frac{mc^2}{\hbar}\varphi\exp(-\frac{i}{\hbar}mc^2t) \\
\frac{\partial^2\psi}{\partial t^2} &= \frac{\partial}{\partial t}\left(\frac{\partial\varphi}{\partial t} - i\frac{mc^2}{\hbar}\varphi\right)\exp(-\frac{i}{\hbar}mc^2t) \\
&\approx \left[-i\frac{mc^2}{\hbar}\frac{\partial\varphi}{\partial t} - i\frac{mc^2}{\hbar}\frac{\partial\varphi}{\partial t} - \frac{m^2c^4}{\hbar^2}\varphi\right]\exp(-\frac{i}{\hbar}mc^2t) \\
&= -\left[2i\frac{mc^2}{\hbar}\frac{\partial\varphi}{\partial t} + \frac{m^2c^4}{\hbar^2}\varphi\right]\exp(-\frac{i}{\hbar}mc^2t)
\end{aligned} \tag{3.19}$$

Inserting this result in (3.15) gives

$$-\frac{1}{c^2}\left[i\frac{2mc^2}{\hbar}\frac{\partial\varphi}{\partial t} + \frac{m^2c^2}{\hbar^2}\varphi\right]\varphi\exp(-\frac{i}{\hbar}mc^2t) = \left[\triangle - \frac{m^2c^4}{\hbar^2}\right]\exp(-\frac{i}{\hbar}mc^2t) \tag{3.20}$$

from which follows

$$i\hbar\frac{\partial\varphi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\varphi. \tag{3.21}$$

This is the free Schrödinger equation for spinless particles. Since the type of particle described by a wave equation does not depend upon whether the particle is relativistic or nonrelativistic, the Klein-Gordon equation describes spin-0 particles.

## 3.3 Free Spin-0 Particles

For discussing the solution of the free Klein-Gordon equation (3.15) we return to the interpretation of the current density (3.13), which we discarded due to $\rho$ given in (3.13) not being positive definite. The probability interpretation is not applicable. However, there is the following alternative: One obtains a *four-current charge density* by multiplying the current density $j_\mu$ in (3.13) with an elementary charge $e$

$$j'_\mu = \frac{ie\hbar}{2m}(\psi^\star \partial_\mu \psi - \psi \partial_\mu \psi^\star), \tag{3.22}$$

where

$$\rho' = \frac{ie\hbar}{2mc^2}\left(\psi^\star \frac{\partial \psi}{\partial t} - \psi \frac{\partial \psi^\star}{\partial t}\right) \tag{3.23}$$

defines the **charge density**, and

$$\mathbf{j}' = \frac{ie\hbar}{2m}\left(\psi^\star \nabla \psi - \psi \nabla \psi^\star\right) \tag{3.24}$$

defines the **charge-current density**. The charge density (3.23) is allowed to be positive, zero, or negative. This is consistent with the existence of particles and antiparticles in the theory.

Let us now calculate the solution for **free particles**. A possible ansatz for the solution for a free wave is given in (3.1)

$$\psi(x) = a \exp\left(-\frac{i}{\hbar} p_\mu x^\mu\right) \tag{3.25}$$

where $1/\hbar p_\mu = k_\mu$. We had seen that because of (3.7) there exist two possible solutions for a given momentum $\mathbf{p}$, one with positive and one with negative energy. Consequently

$$\psi_\pm(x) = a_\pm \exp(\frac{i}{\hbar}(\mathbf{p}\cdot\mathbf{x} \mp |E_p|t)), \tag{3.26}$$

where $E_p = \pm c\sqrt{\mathbf{p}^2 + m^2c^2}$. Inserting this into the expression for the density (3.23) gives

$$\rho_\pm = \pm \frac{e|E_p|}{mc^2} \psi^\star_\pm \psi_\pm. \tag{3.27}$$

This suggests the following interpretation: $\psi_+$ specifies particles with charge $+e$ and $\psi_-$ specifies particles with the same mass, but with charge $-e$. The general solution of the wave equation will always be a superposition of both types of functions.

Let us now discretize the continuous plane wave by confining the wave to a cubic box (normalization box) with box length $L$ and demand periodic boundary conditions at the box walls. This leads to

$$\psi_{n(\pm)} = A_{n(\pm)} \exp\left[\frac{i}{\hbar}(\mathbf{p}_n \cdot \mathbf{x} \mp E_p n t)\right], \tag{3.28}$$

where

$$\mathbf{p}_n = \frac{2\pi}{L} n, \quad n = (n_1, n_2, n_3), \quad n_i \in \mathcal{N} \tag{3.29}$$

and

$$E_p n = c\sqrt{p_n^2 + m^2 c^2} \equiv E_n. \tag{3.30}$$

Here $n$ is a (discrete) vector in the lattice space with axes $n_1, n_2, n_3$. With (3.27) the normalization factors $A_{n(\pm)}$ are determined by the requirement that

$$\pm \int_{L^3} d^3x \rho_\pm(\mathbf{x}) = \pm \frac{eE_n}{mc^2} |A_{n(\pm)}|^2 L^3. \tag{3.31}$$

Choosing the phase such that the amplitudes are real,

$$A_{n(\pm)} = \sqrt{\frac{mc^2}{L^3 E_n}} \tag{3.32}$$

and thus

$$\psi_{n(\pm)} = \sqrt{\frac{mc^2}{L^3 E_n}} \exp\left[\frac{i}{\hbar}(\mathbf{p}_n \cdot \mathbf{x} \mp E_n t)\right]. \tag{3.33}$$

The most general solution of the Klein-Gordon equation for positive/negative energy spin-0 particles is then given by

$$\begin{aligned} \psi_+ &= \sum_n a_n \psi_{n(+)} = \sum_n a_n \sqrt{\frac{mc^2}{L^3 E_n}} \exp\left[\frac{i}{\hbar}(\mathbf{p}_n \cdot \mathbf{x} - E_n t)\right] \\ \psi_- &= \sum_n a_n \psi_{n(-)} = \sum_n a_n \sqrt{\frac{mc^2}{L^3 E_n}} \exp\left[\frac{i}{\hbar}(\mathbf{p}_n \cdot \mathbf{x} + E_n t)\right]. \end{aligned} \tag{3.34}$$

For neutral particles the Klein-Gordon field $\psi$ has to be real, see (3.23), i.e. $\psi^\star = \psi$. Thus the wave for a neutral particle can be constructed as

$$\begin{aligned} \psi_{n(0)} &= \frac{1}{\sqrt{2}}\left(\psi_{n(+)}(p_n) + \psi_{n(-)}(-p_n)\right) \\ &= \sqrt{\frac{mc^2}{2L^3 E_n}}\left(\exp\left[\frac{i}{\hbar}(\mathbf{p}_n \cdot \mathbf{x} - E_n t)\right] + \exp\left[\frac{-i}{\hbar}(\mathbf{p}_n \cdot \mathbf{x} + E_n t)\right]\right) \\ &= \sqrt{\frac{mc^2}{2L^3 E_n}}\, 2\cos\left(\frac{1}{\hbar}(\mathbf{p}_n \cdot \mathbf{x} - E_n t)\right). \end{aligned} \tag{3.35}$$

Thus, with $\psi_{n(0)} = \psi^{\star}_{n(0)}$ follows $\rho' = 0$ and $\mathbf{j}'(\mathbf{x}, t) = 0$. Consequently, in this case there is no conservation law.

The previous showed that relativistic quantum theory leads to new degrees of freedom of particles. In a nonrelativistic theory, free spinless particles can propagate freely with a well defined momentum $\mathbf{p}$. In the relativistic case of free spinless particles, there exist three solutions, which correspond to the electric charge (+,-,0) of the particles, for every momentum $\mathbf{p}$.

## 3.4 The Charged Klein-Gordon Field

In case of a complex, i.e. charged scalar field, the current is given through (3.22) with $\partial j^{\mu}/\partial x^{\mu} = 0$ and a total charge

$$Q = \frac{ie\hbar}{2mc^2} \int d^3x \left( \varphi^{\star} \frac{\partial \varphi}{\partial t} - \varphi \frac{\partial \varphi^{\star}}{\partial t} \right). \tag{3.36}$$

To examine charged fields in some more detail, we decompose $\varphi(x)$ into real and imaginary components

$$\varphi(x) = \frac{1}{\sqrt{2}} \left( \varphi_1(x) + i\varphi_2(x) \right), \tag{3.37}$$

where $\varphi_1(x)$ and $\varphi_2(x)$ are real. If $\varphi(x)$ fulfills the Klein-Gordon equation, so do the components $\varphi_1(x)$ and $\varphi_2(x)$.

Conversely, the following is true: If two fields $\varphi_1(x)$ and $\varphi_2(x)$ separately fulfill a Klein-Gordon equation with the same mass $m = m_1 = m_2$, then the equations can be replaced by **one** equation for a complex field, i.e.

$$\begin{aligned} \varphi &= \frac{1}{\sqrt{2}}(\varphi_1 + i\varphi_2) \\ \varphi^{\star} &= \frac{1}{\sqrt{2}}(\varphi_1 - i\varphi_2) \end{aligned} \tag{3.38}$$

with

$$\begin{aligned} \left( \Box + \frac{m^2c^2}{\hbar^2} \right) \varphi = 0 \\ \left( \Box + \frac{m^2c^2}{\hbar^2} \right) \varphi^{\star} = 0 \end{aligned} \tag{3.39}$$

By interchanging $\varphi$ and $\varphi^{\star}$ in (3.36). we obtain the opposite charge. Hence $\varphi$ and $\varphi^{\star}$ *characterize opposite charges.* These studies can, e.g., be applied to the pion triplet $(\pi^+, \pi^-, \pi^0)$.

## 3.5 The Klein-Gordon Equation in Schrödinger Form

To demonstrate the new degree of freedom (charge) in a more distinct way, it is advantageous to transform the Klein-Gordon equation (3.15), which is second order in time, into two coupled differential equations which are first order in time. this is achieved by the ansatz

$$\begin{aligned} \psi &= \varphi + \chi \\ i\hbar\frac{\partial\psi}{\partial t} &= mc^2(\varphi - \chi) \end{aligned} \tag{3.40}$$

in which $\psi$ and $\frac{\partial\psi}{\partial t}$ are expressed as linear combination of $\varphi$ and $\chi$. The two coupled differential equations

$$\begin{aligned} i\hbar\frac{\partial\varphi}{\partial t} &= -\frac{\hbar^2}{2m}\triangle(\varphi + \chi) + mc^2\varphi \\ i\hbar\frac{\partial\chi}{\partial t} &= \frac{\hbar^2}{2m}\triangle(\varphi + \chi) - mc^2\chi \end{aligned} \tag{3.41}$$

are equivalent to the Klein-Gordon equation (3.15), as can be shown by adding and subtracting the two equations of (3.41).
Addition gives

$$i\hbar\frac{\partial}{\partial t}(\varphi + \chi) = mc^2(\varphi - \chi), \tag{3.42}$$

which leads to the trivial identity $\partial\psi/\partial t = \partial\psi/\partial t$.
Subtraction gives

$$i\hbar\frac{\partial}{\partial t}(\varphi - \chi) = -\frac{\hbar^2}{2m}\triangle(\varphi + \chi) + mc^2(\varphi + \chi). \tag{3.43}$$

With (3.40) one obtains

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\left(\frac{i\hbar}{mc^2}\frac{\partial\psi}{\partial t}\right) &= -\frac{\hbar^2}{2m}\triangle\psi + mc^2\psi \\ -\frac{\hbar^2}{mc^2}\frac{\partial^2\psi}{\partial t^2} &= -\frac{\hbar^2}{2m}\triangle\psi + mc^2\psi \\ \frac{1}{c^2}\frac{\partial^2\psi}{\partial t^2} &= \triangle\psi - \frac{m^2c^2}{\hbar^2}\psi, \end{aligned} \tag{3.44}$$

which is just the Klein-Gordon equation.

The coupled equations can be written in a more compact form. For this we introduce

$$\Psi = \begin{pmatrix} \varphi \\ \chi \end{pmatrix} \tag{3.45}$$

and make use of the Pauli matrices, $\hat{\tau}_i$, $\mathbf{1}$. However, here they do not act in spin-space, but rather in the space introduced by (3.45). With this the coupled equations (3.41) can be combined in a Schrödinger type equation

$$i\hbar\frac{\partial\Psi}{\partial t} = \hat{H}_f\Psi, \tag{3.46}$$

where the Hamiltonian $\hat{H}_f$ for free particles is given by

$$\begin{aligned} \hat{H}_f &= (\hat{\tau}_3 + i\hat{\tau}_2)\frac{\hat{p}^2}{2m} + \hat{\tau}_3 mc^2 \\ &= \begin{pmatrix} 1 & 1 \\ -1 & -1 \end{pmatrix}\frac{\hat{p}^2}{2m} + \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} mc^2. \end{aligned} \tag{3.47}$$

Each component of the vector $\Psi$ individually satisfies the Klein-Gordon equation. From (3.46) follows

$$\begin{aligned} \left(i\hbar\frac{\partial}{\partial t} + \hat{H}_f\right)\left(i\hbar\frac{\partial}{\partial t} - \hat{H}_f\right) &= 0 \\ \left(-\hbar^2\frac{\partial^2}{\partial t^2} - \hat{H}_f^2\right) &= 0 \end{aligned} \tag{3.48}$$

With $\hat{H}_f^2 = c\hat{p}^2 + m^2c^4$ follows

$$\left(-\hbar^2\frac{\partial^2}{\partial t^2} - \hbar^2c^2\triangle - m^2c^4\right)\Psi = 0, \tag{3.49}$$

which is just the Klein-Gordon equation valid for each component of $\Psi$. With this representation, the expression for the density becomes especially simple. From (3.23) using (3.40) one obtains

$$\begin{aligned} \rho' &= \frac{ie\hbar}{2mc^2}\left(\psi^\star\frac{\partial\psi}{\partial t} - \psi\frac{\partial\psi^\star}{\partial t}\right) \\ &= \frac{emc^2}{2mc^2}\left(\psi^\star(\varphi-\chi) + \psi(\varphi^\star-\chi^\star)\right) \\ &= \frac{e}{2}\left((\varphi^\star+\chi^\star)(\varphi-\chi) + (\varphi+\chi)(\varphi^\star-\chi^\star)\right) \\ &= \frac{e}{2}(\varphi^\star\varphi - \chi^\star\chi) \\ &= e\Psi^\dagger\hat{\tau}_3\Psi. \end{aligned} \tag{3.50}$$

Similarly, the current vector is given in Schrödinger representation as

$$\mathbf{j}' = \frac{e\hbar}{2mi}\left(\Psi^\dagger\hat{\tau}_3(\hat{\tau}_3 + i\hat{\tau}_2)\nabla\Psi - (\nabla\Psi^\dagger)\hat{\tau}_3(\hat{\tau}_3 + i\hat{\tau}_2)\Psi\right). \tag{3.51}$$

The normalization is given by

$$\begin{aligned}\int d^3x\Psi^\dagger)\hat{\tau}_3\Psi &= \int d^3x(\varphi^\star\varphi - \chi^\star\chi) = \pm 1 \\ \int d^3x\rho'(\mathbf{x}) &= \pm e.\end{aligned} \tag{3.52}$$

Let us consider free particles in this representation and write

$$\Psi = \begin{pmatrix} \varphi \\ \chi \end{pmatrix} = A\begin{pmatrix} \varphi_0 \\ \chi_0 \end{pmatrix} \exp\left[\frac{i}{\hbar}(\mathbf{p}\cdot\mathbf{x} - Et)\right] \tag{3.53}$$

and substitute this ansatz into (3.47) and find

$$E\begin{pmatrix} \varphi \\ \chi \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ -1 & -1 \end{pmatrix}\frac{\hat{p}^2}{2m}\begin{pmatrix} \varphi \\ \chi \end{pmatrix} + \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} mc^2 \begin{pmatrix} \varphi \\ \chi \end{pmatrix} \tag{3.54}$$

which gives the two separate equations

$$\begin{aligned} E\varphi &= \frac{\hat{p}^2}{2m}(\varphi + \chi) + mc^2\varphi \\ E\chi &= -\frac{\hat{p}^2}{2m}(\varphi + \chi) - mc^2\chi \end{aligned} \tag{3.55}$$

$\varphi_0$ and $\chi_0$ are therefore determined by the solution of the coupled equations

$$\begin{aligned} \left(E - \frac{\hat{p}^2}{2m} - mc^2\right)\varphi_0 - \frac{\hat{p}^2}{2m}\chi_0 &= 0 \\ \frac{\hat{p}^2}{2m}\varphi_0 + \left(E + \frac{\hat{p}^2}{2m} + mc^2\right)\chi_0 &= 0 \end{aligned} \tag{3.56}$$

Since the determinant of the system (3.56) needs to vanish, it follows that

$$E^2 - \left(\frac{\hat{p}^2}{2m} + mc^2\right)^2 + \left(\frac{\hat{p}^2}{2m}\right)^2 = 0, \tag{3.57}$$

from which one recoveries the relativistic energy momentum relation

$$E = \pm c\sqrt{p^2 + mc^2} \equiv \pm E_p. \tag{3.58}$$

Consider the positive energy solution $E = +E_p$:
From (3.53) we obtain

$$\Psi^{(+)}(\mathbf{p}) = A_{(+)}\begin{pmatrix} \varphi_0^{(+)} \\ \chi_0^{(+)} \end{pmatrix} \exp\left[\frac{i}{\hbar}(\mathbf{p}\cdot\mathbf{x} - E_pt)\right] \equiv \begin{pmatrix} \varphi^{(+)}(\mathbf{p}) \\ \chi^{(+)}(\mathbf{p}) \end{pmatrix} \tag{3.59}$$

From (3.55) follows that

$$\begin{aligned} (E_p - mc^2)\varphi_0^{(+)} &= -(E_p + mc^2)\chi_0^{(+)} \\ \varphi_0^{(+)} &= \frac{mc^2 + E_p}{mc^2 - E_p}\chi_0^{(+)} \end{aligned} \tag{3.60}$$

so that, when choosing $\chi_0^{(+)} = mc^2 - E_p$, it follows that

$$\begin{pmatrix} \varphi_0^{(+)} \\ \chi_0^{(+)} \end{pmatrix} = \begin{pmatrix} mc^2 + E_p \\ mc^2 - E_p \end{pmatrix}. \tag{3.61}$$

Eq. (3.52) allows to calculate the normalization constant $A_{(+)}$ from

$$|A_{(+)}|^2 \int d^3x (\varphi_0^{(+)\star}\varphi_0^{(+)} - \chi_0^{(+)\star}\chi_0^{(+)}) = |A_{(+)}|^2 L^3 \left[(mc^2 + E_p)^2 - (mc^2 - E_p)^2\right] = 1 \tag{3.62}$$

If the phase is chosen to be real, then

$$A_{(+)} = \frac{1}{\sqrt{4mc^2}\sqrt{L^3 E_p}}. \tag{3.63}$$

In the other case, $E = -E_p$, proceeding similarly leads to the wave function

$$\Psi^{(-)}(\mathbf{p}) = A_{(-)} \begin{pmatrix} \varphi_0^{(-)} \\ \chi_0^{(-)} \end{pmatrix} \exp\left[\frac{i}{\hbar}(\mathbf{p}\cdot\mathbf{x} + E_p t)\right] \equiv \begin{pmatrix} \varphi^{(-)}(\mathbf{p}) \\ \chi^{(-)}(\mathbf{p}) \end{pmatrix} \tag{3.64}$$

with

$$\begin{pmatrix} \varphi_0^{(-)} \\ \chi_0^{(-)} \end{pmatrix} = \begin{pmatrix} mc^2 - E_p \\ mc^2 + E_p \end{pmatrix} \tag{3.65}$$

and $A_{(-)} = A_{(+)}$.

Consider the nonrelativistic limit, where $E_p \approx mc^2 + \frac{p^2}{2m}$. Then

$$\begin{aligned} \begin{pmatrix} A_{(+)}\varphi_0^{(+)} \\ A_{(+)}\chi_0^{(+)} \end{pmatrix} &= \frac{1}{\sqrt{L^3}} \begin{pmatrix} (mc^2 + E_p)/\sqrt{4E_p mc^2} \\ (mc^2 - E_p)/\sqrt{4E_p mc^2} \end{pmatrix} \\ &\approx \frac{1}{\sqrt{L^3}} \begin{pmatrix} 2mc^2/2mc^2 \\ (-\frac{p^2}{2m})/2mc^2 \end{pmatrix} \\ &= \frac{1}{\sqrt{L^3}} \begin{pmatrix} 1 \\ -1/4(v/c)^2 \end{pmatrix} \stackrel{v/c\to 0}{\longrightarrow} \frac{1}{\sqrt{L^3}} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \end{aligned} \tag{3.66}$$

Similarly

$$\begin{pmatrix} A_{(-)}\varphi_0^{(-)} \\ A_{(-)}\chi_0^{(-)} \end{pmatrix} \approx \frac{1}{\sqrt{L^3}} \begin{pmatrix} -1/4(v/c)^2 \\ 1 \end{pmatrix} \stackrel{v/c\to 0}{\longrightarrow} \frac{1}{\sqrt{L^3}} \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{3.67}$$

Thus, we see that in the nonrelativistic limit for states with positive charge the upper component is large, and the lower one is small. For negative energies, we find the reverse being true.

Charge conjugation follows in this case from comparing the expressions for the wave functions in 3.59 for $\Psi^{(+)}(\mathbf{p})$ with the corresponding expression for $\Psi^{(-)}(\mathbf{p})$, 3.64.

$$\Psi^{(-)}(\mathbf{p} = \begin{pmatrix} \varphi^{(-)}(-\mathbf{p}) \\ \chi^{(-)}(-\mathbf{p}) \end{pmatrix} = \begin{pmatrix} \chi^{(+)\star}(\mathbf{p}) \\ \varphi^{(-)\star}(\mathbf{p}) \end{pmatrix} = \tau_1 \Psi^{(+)\star}(\mathbf{p}). \tag{3.68}$$

Thus, if

$$\Psi \equiv \begin{pmatrix} \varphi \\ \chi \end{pmatrix} \tag{3.69}$$

represents a positive charge, then the state

$$\hat{C}\Psi\hat{C}^{-1} \equiv \Psi_C = \tau_1 \Psi^\star = \begin{pmatrix} \chi^\star \\ \varphi^\star \end{pmatrix} \tag{3.70}$$

describes a particle with negative charge. Thus, $\Psi_C$ is the charge-conjugate state of $\Psi$. Similarly,

$$(\Psi_C)_C = \tau_1(\tau_1\Psi^\star)^\star = \Psi, \tag{3.71}$$

i.e. $\Psi$ is the **charge-conjugate** state of $\Psi_C$.

Explicitly, charge conjugation implies the following transformations

$$\begin{aligned} \varphi_0^{(+)} &\rightarrow \chi_0^{(-)} \\ \chi_0^{(+)} &\rightarrow \varphi_0^{(-)} \\ \mathbf{p} &\rightarrow -\mathbf{p} \\ +E_p &\rightarrow -E_p \end{aligned} \tag{3.72}$$

If the state $\Psi$ describes a **particle**, then $\Psi_C$ describes the corresponding **antiparticle**. (Example: $\pi^+$ and $\pi^-$)

Neutral particles fulfill the requirement that they are charge-conjugate states to themselves, i.e.

$$\Psi_C = \tau_1 \Psi^\star = \alpha\Psi, \tag{3.73}$$

where $\alpha$ has to be real. Remember, that the Klein-Gordon wave function $\Psi = \varphi + \chi$ has to be real. Thus, $\Im\varphi = -\Im\chi$ has to hold, as well as $\Im(\alpha\varphi) = \Im(\alpha\chi)$, which can only be true if $\alpha$ real. From $(\Psi_C)_C = \Psi$ follows that

$$(\alpha\Psi)_C = \tau_1(\alpha\Psi)^\star = \alpha\tau_1\Psi^\star = \alpha\alpha\Psi = \Psi, \tag{3.74}$$

so that

$$\alpha^2 = 1 \quad ; \quad \alpha = \pm 1. \tag{3.75}$$

Thus there exist two different kinds of neutral particles. To resolve this, one introduces a new quantum number, the **charge parity** $\alpha$. One has then

(a) Neutral particles with **positive** charge parity ($\alpha = +1$)

$$\Psi_C = \tau_1 \Psi^\star = \Psi \;\; or \;\; \varphi^\star = \chi$$

(b) Neutral particles with **negative** charge parity ($\alpha = -1$)

$$\Psi_C = \tau_1 \Psi^\star = -\Psi \;\; or \;\; \varphi^\star = -\chi$$

## 3.6 Free Spin-0 Particles in the Feshbach-Villard Representation

The nonrelativistic limit of (3.66) and (3.67) indicate that positively charged particles have in this limit a large upper component ($|\varphi^{(+)}| \gg |\chi^{(+)}|$), while negatively charged particles have a large lower component ($|\chi^{(-)}| \gg |\varphi^{(-)}|$). It is tempting to find a representation in which positve and negative energy solutions always take the form

$$\begin{aligned} \phi^{(+)}(\mathbf{p}) &\equiv u(\mathbf{p}) \sim \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ \phi^{(-)}(\mathbf{p}) &\equiv v(\mathbf{p}) \sim \begin{pmatrix} 0 \\ 1 \end{pmatrix} \end{aligned} \tag{3.76}$$

Such a representation was presented by H. Feshbach and F. Villard (Rev. Mod. Phys. **30**, 24 (1958)). It can be established by a transformation

$$\begin{aligned} \phi &= \hat{U}\Psi \\ \phi^\dagger &= \Psi^\dagger \hat{U}^\dagger, \end{aligned} \tag{3.77}$$

where $\hat{U}$ is given by

$$\begin{aligned} \hat{U} &= \frac{1}{\sqrt{4mc^2E_p}} \begin{pmatrix} (mc^2+E_p) & -(mc^2-E_p) \\ -(mc^2-E_p) & (mc^2+E_p) \end{pmatrix} \\ &= \mathbf{1}\frac{1}{\sqrt{4mc^2E_p}} \Big( (mc^2+E_p) - \tau_1(mc^2-E_p) \Big) . \end{aligned} \tag{3.78}$$

First, consider the effect of $\hat{U}$ applied on the states $\Psi^{(+)}(\mathbf{p})$ of (3.59) and $\Psi^{(-)}(\mathbf{p})$ of (3.64)

$$\begin{aligned}
\phi^{(+)}(\mathbf{p}) &= \hat{U}\Psi^{(+)}(\mathbf{p}) \\
&= \hat{U}\frac{1}{\sqrt{L^3}}\frac{1}{\sqrt{4mc^2E_p}}\begin{pmatrix} mc^2+E_p \\ mc^2-E_p \end{pmatrix}\exp\left[\frac{i}{\hbar}(\mathbf{p}\cdot\mathbf{x}-E_pt)\right] \\
&= \frac{1}{\sqrt{L^3}}\frac{1}{\sqrt{4mc^2E_p}}\begin{pmatrix} (mc^2+E_p) & -(mc^2-E_p) \\ -(mc^2-E_p) & (mc^2+E_p) \end{pmatrix}\begin{pmatrix} mc^2+E_p \\ mc^2-E_p \end{pmatrix}\exp\left[\frac{i}{\hbar}(\mathbf{p}\cdot\mathbf{x}-E_pt)\right] \\
&= \frac{1}{\sqrt{L^3}}\begin{pmatrix} 1 \\ 0 \end{pmatrix}\exp\left[\frac{i}{\hbar}(\mathbf{p}\cdot\mathbf{x}-E_pt)\right]. \qquad (3.79)
\end{aligned}$$

Similarly,

$$\begin{aligned}
\phi^{(-)}(\mathbf{p}) &= \hat{U}\Psi^{(-)}(\mathbf{p}) \\
&= \hat{U}\frac{1}{\sqrt{L^3}}\frac{1}{\sqrt{4mc^2E_p}}\begin{pmatrix} mc^2-E_p \\ mc^2+E_p \end{pmatrix}\exp\left[\frac{i}{\hbar}(\mathbf{p}\cdot\mathbf{x}+E_pt)\right] \\
&= \frac{1}{\sqrt{L^3}}\begin{pmatrix} 0 \\ 1 \end{pmatrix}\exp\left[\frac{i}{\hbar}(\mathbf{p}\cdot\mathbf{x}+E_pt)\right]. \qquad (3.80)
\end{aligned}$$

So, $\hat{U}$ is the desired transformation. However, $\hat{U}$ is not unitary in the usual sense (i.e. $\hat{U}^{-1} \neq \hat{U}^\dagger$), since

$$\hat{U}^{-1} = \tau_3\hat{U}\tau_3 = \mathbf{1}\frac{1}{\sqrt{4mc^2E_p}}\left[(mc^2+E_p)+\tau_1(mc^2-E_p)\right]. \qquad (3.81)$$

By explicit calculation we see that

$$\hat{U}\hat{U}^{-1} = \mathbf{1}. \qquad (3.82)$$

The normalization of the $\phi^{(\pm)}$-functions follows from the normalization of $\Psi^{(\pm)}$ (3.52) as

$$\begin{aligned}
\pm 1 &= \int d^3x\Psi^\dagger\tau_3\Psi \\
&= \int d^3x(\hat{U}^{-1}\phi)^\dagger\tau_3(\hat{U}^{-1}\phi) \\
&= \int d^3x\phi^\dagger(\hat{U}^{-1})^\dagger\tau_3\hat{U}^{-1}\phi \\
&= \int d^3x\phi^\dagger\tau_3\phi \qquad (3.83)
\end{aligned}$$

Here we used that from (3.81) follows $\tau_3\hat{U}^{-1} = \hat{U}\tau_3$ and thus

$$(\hat{U}^{-1})^\dagger\tau_3\hat{U}^{-1} = (\hat{U}^{-1})^\dagger\hat{U}\tau_3 = \hat{U}^{-1}\hat{U}\tau_3 = \tau_3 \qquad (3.84)$$

Thus, we can define a generalized scalar product

$$\langle\Psi|\Psi'\rangle_\phi \equiv \int d^3x \Psi^\dagger \tau_3 \Psi \tag{3.85}$$

so that from (3.83) follows

$$\langle\Psi|\Psi'\rangle_\phi = \langle\phi|\phi'\rangle_\phi, \tag{3.86}$$

i.e. the generalized scalar product is invariant under the transformation $\hat{U}$. It seems natural to call an operator $\hat{A}$ with the property

$$\langle\Psi|\Psi'\rangle_\phi = \langle\hat{A}\phi|\hat{A}\phi'\rangle_\phi \tag{3.87}$$

**$\phi$-unitary**. Such an operator fulfills the condition

$$\hat{A}^H \equiv \tau_3 \hat{A}^\dagger \tau_3 = \hat{A}^{-1}. \tag{3.88}$$

Since

$$\int d^3x \Psi^\dagger \tau_3 \Psi' = \int d^3x \phi^\dagger \hat{A}^\dagger \tau_3 \hat{A} \phi', \tag{3.89}$$

and thus

$$\begin{aligned} \hat{A}^\dagger \tau_3 \hat{A} &= \tau_3 \\ \tau_3 \hat{A}^\dagger \tau_3 \hat{A} &= \mathbf{1} \end{aligned} \tag{3.90}$$

and thus $\tau_3 \hat{A}^\dagger \tau_3 = \hat{A}^{-1}$ as required in (3.88). If $\hat{A}$ and $\tau_3$ commute, then $\hat{A}^\dagger = \hat{A}$ follows from (3.88), i.e. the normal unitarity relation. With this the charge $Q$ of a state $\Psi$ can be written as

$$Q = e \int d^3x \Psi^\dagger \tau_3 \Psi = e\langle\Psi|\Psi\rangle_\phi \tag{3.91}$$

The free Hamiltonian $\hat{H}_f$ from (3.47) takes in the Feshbach-Villard representation a particular simple form,

$$\hat{H}_\phi = \hat{U}\hat{H}_f\hat{U}^{-1} = \tau_3 E_p, \tag{3.92}$$

which can be shown by explicit calculation.

Thus the Klein-Gordon equation given in (3.46) as

$$i\hbar\frac{\partial\Psi}{\partial t} = \hat{H}_f\Psi \tag{3.93}$$

can be transformed by multiplication with $\hat{U}$ from the left to

$$\begin{aligned} i\hbar\frac{\partial\hat{U}\Psi}{\partial t} &= \hat{U}\hat{H}_f\hat{U}^{-1}\hat{U}\Psi \\ i\hbar\frac{\partial\phi}{\partial t} &= \tau_3 E_p \phi \end{aligned} \tag{3.94}$$

which is the Klein-Gordon equation in the Feshbach-Villard representation. This equation has two different solutions for any given momentum $\mathbf{p}$, namely one with $+E_p$ and one with $-E_p$.

A direct solution of (3.94) can be found by the ansatz

$$\phi = \exp\left[\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{x}\right]\theta \tag{3.95}$$

with

$$\theta = \begin{pmatrix} \theta_1 \\ \theta_2 \end{pmatrix}. \tag{3.96}$$

Inserting this in (3.94) gives

$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix} \theta_1 \\ \theta_2 \end{pmatrix} = E_p\begin{pmatrix} \theta_1 \\ -\theta_2 \end{pmatrix} \tag{3.97}$$

and thus

$$\begin{aligned} i\hbar\frac{\partial\theta_1}{\partial t} &= E_p\theta_1 \\ i\hbar\frac{\partial\theta_2}{\partial t} &= -E_p\theta_2. \end{aligned} \tag{3.98}$$

Integration gives

$$\begin{aligned} \theta_1 &= N_1\exp\left[-\frac{i}{\hbar}E_p t\right] \\ \theta_2 &= N_2\exp\left[\frac{i}{\hbar}E_p t\right]. \end{aligned} \tag{3.99}$$

Here $N_1$ and $N_2$ are normalization constants which are determined by the normalization condition (3.83) as

$$\int d^3x\phi^\dagger\tau_3\phi = \int d^3x\theta^\dagger\tau_3\theta = \pm 1 \tag{3.100}$$

yielding

$$|N_1|^2 - |N_2|^2 = \pm\frac{1}{V}. \tag{3.101}$$

This lead to the two independent solutions

$$\begin{aligned} \phi^{(+)} &= \frac{1}{\sqrt{V}}\begin{pmatrix} 1 \\ 0 \end{pmatrix}\exp\left[\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{x} - E_p t\right] \quad \textit{charge} + \textit{1} \\ \phi^{(-)} &= \frac{1}{\sqrt{V}}\begin{pmatrix} 0 \\ 1 \end{pmatrix}\exp\left[\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{x} + E_p t\right] \quad \textit{charge} - \textit{1} \end{aligned} \tag{3.102}$$

and each linear combination of type

$$n_1 \phi^{(+)} + n_2 \phi^{(-)} \tag{3.103}$$

with $|n_1|^2 - |n_2|^2 = 1$ being a normalized eigenfunction of the momentum $\mathbf{p}$ with charge $+1$ and each linear combination with $|n_1|^2 - |n_2|^2 = -1$ being a normalized solution with charge -1.

## 3.7 Interpretation of One-Particle Operators in Relativistic Quantum Mechanics

The Schrödinger form of the free Klein-Gordon equation was given in (3.46) as

$$i\hbar \frac{\partial \Psi}{\partial t} = \hat{H}_f \Psi \tag{3.104}$$

with

$$\Psi(\vec{x}, t) = \begin{pmatrix} \phi(\vec{x}, t) \\ \chi(\vec{x}, t) \end{pmatrix} \tag{3.105}$$

and the free Hamiltonian

$$\hat{H}_f = (\hat{\tau}_3 + i\hat{\tau}_2) \frac{\hat{p}^2}{2m} + mc^2 \hat{\tau}_3 . \tag{3.106}$$

With the help of (3.104) the vector $\Psi(\vec{x}, t)$ may be evaluated at any later time $t$, if the values $\Psi(\vec{x}, 0)$ are known at $t = 0$. This can be expressed by the transformation

$$\Psi(\vec{x}, t) = \hat{U}(t) \Psi(\vec{x}, 0) \tag{3.107}$$

with

$$\hat{U}(t) = \exp\left(-\frac{i}{\hbar} \hat{H}_f t\right) = \mathbf{1} + \left(-\frac{i\hat{H}_f}{\hbar}\right) t + \left(-\frac{i\hat{H}_f}{\hbar}\right)^2 \frac{t^2}{2!} = \cdots \tag{3.108}$$

As in non-relativistic quantum mechanics, time dependence may either be expressed by the state vectors $\Psi(\vec{x}, t)$ (Schrödinger picture) or can be incorporated in the operators

(Heisenberg picture). The change from the Schrödinger to Heisenberg picture is performed by the transformations

$$
\begin{aligned}
\Psi_H(\vec{x}) &= \hat{U}(t)\ \Psi(\vec{x},t) \\
\hat{F}_H(t) &= \hat{U}^{-1}(t)\ \hat{F}(0)\ \hat{U}(t)
\end{aligned}
\tag{3.109}
$$

which leave the scalar product invariant.

$$
\begin{aligned}
\langle \Psi(\vec{x},t)\ |\hat{F}(0)|\ \Psi'(\vec{x},t)) \rangle &= \langle \hat{U}(t)\ \Psi_H(\vec{x}\ |\hat{F}(0)|\ \hat{U}(t)\ \Psi'_H(\hat{x})\rangle \\
&= \langle \Psi_H(\hat{x})\ |\hat{U}^{-1}\ \hat{F}(0)|\ \Psi'_H\ (\hat{x})\rangle \\
&= \langle \Psi_H(\hat{x})\ |\hat{F}_H(t)|\ \Psi'_H\hat{x})\rangle\ .
\end{aligned}
\tag{3.110}
$$

For the time independent $\hat{H}_f$ of (3.106) follows

$$
\begin{aligned}
i\hbar\ \frac{d\hat{F}}{dt} &= i\hbar\ \frac{d}{dt}\ \left( e^{i\hat{H}_f\ t/\hbar}\ \hat{F}(0)\ e^{-i\hat{H}_f\ t/\hbar} \right) \\
&= -\hat{H}_f\ \hat{F}\ +\ \hat{F}\ \hat{H}_f\ =\ [\hat{F}, \hat{H}_f]
\end{aligned}
\tag{3.111}
$$

in analogy to non-relativistic quantum mechanics. From (3.112) follows that the physical observation $F$ whose corresponding operator $\hat{F}$ commutes with $\hat{H}_f$, are constants of motion. This means that the expectation values of these operators are constant in time. One of the basic postulates in non-relativistic quantum mechanics states that the eigenvalues of an operator describe the measurable values of the corresponding physical quantity in a state of the system. To satisfy this postulate in the relativistic theory, we must modify the definitions of some of the operators.

Let us consider the energy of a system. The eigenvalues and eigenstates of the operator $\hat{H}_f$ (3.106) are determined (in case of the free motion with momentum $\vec{p}$) by

$$
\hat{H}_f \Psi\ =\ E\Psi\ .
\tag{3.112}
$$

The free motion had two solutions (see previous section)

$$\Psi_\lambda(\vec{x}) \;=\; \frac{1}{\sqrt{2^3}} \begin{pmatrix} \varphi_0^\lambda \\ \chi_0^\lambda \end{pmatrix} \exp\left(\frac{i}{\hbar}\,(\vec{p}\cdot\vec{x})\right) \quad ; \quad \lambda \;=\; \pm\,1 \tag{3.113}$$

for the corresponding energies

$$E_\lambda \;=\; \lambda\; E_p \;=\; \lambda c\,\sqrt{p^2+mc^2}\;. \tag{3.114}$$

$E_{-1}$ is negative and thus can **not** be interpreted as a one-particle energy, which must always be positive. Here we need to remember the double meaning of the energy eigenvalues of the Hamiltonian in non-relativistic quantum mechanics: First, they represent the energy of stationary states. Second, they characterize the time-evolution of the wave function. We have already seen (3.53) that the eigenvalues $E_\lambda$ of $\hat{H}_f$ represent the time dependence of the wave functions in a relativistic theory (factor $\exp\left[-\frac{i}{\hbar}E_pt\right]$), i.e.,

$$\Psi_\lambda(\vec{x},t) \;= \exp\left[-\frac{i}{\hbar}\;\hat{H}_f t\right]\;\Psi_\lambda(\vec{x}) \;=\; \exp\left[-\;\frac{i}{\hbar}\;\lambda\;E_p t\right]\;\Psi_\lambda(\vec{x})\;. \tag{3.115}$$

The energy of these states is always positive and hence $\lambda$ independent. We can see this from the following. The energy $\varepsilon$ of a system in a stationary state is identical with the mean value of the energy, i.e.,

$$\varepsilon_\lambda \;=\; \int d^3x\;\Psi_\lambda^\dagger\;\hat{\tau}_3\;\hat{H}_f\;\Psi_\lambda\;. \tag{3.116}$$

With $\hat{H}_f\Psi_\lambda = E_\lambda\Psi_\lambda = \lambda E_p\Psi_\lambda$ and $\int d^3x\Psi_\lambda^\dagger\hat{\tau}_3\Psi_\lambda = \lambda$, we have

$$\varepsilon_\lambda \;=\; \lambda\;E_p\;\int d^3x\;\Psi_\lambda^\dagger\;\hat{\tau}_3\;\Psi_\lambda \;=\; \lambda^2\;E_p \;=\; E_p\;. \tag{3.117}$$

The energy is always positive and independent of $\lambda$. Thus, the problem of the energy is solved. The dual character of the eigenvalues of $\hat{H}_f$, i.e., as the characteristic factor of the time-evolution and as an energy, evolves quite naturally in the relativistic quantum theory. We can give the correct interpretation of the energies of the states by making use of the canonical formalism, the energy operator is **not** $\hat{H}_f$ but $\hat{\tau}_3\;\hat{H}_f$ (3.116)

In non-relativistic quantum mechanics, there is always a correspondence between a relation of operators and that of classical objects (measurable values). Example: Newton's equation of motion corresponds to the operator equation

$$\frac{d\hat{p}}{dt} = \frac{1}{i\hbar}\,[\hat{p},\hat{H}] \tag{3.118}$$

with $\hat{H} = \frac{\hat{p}^2}{2m} + U(\vec{x})$, or

$$\frac{d\vec{x}}{dt} = \frac{i}{i\hbar}\,[\hat{x}_1,\hat{H}] = \frac{\vec{p}}{m}\ , \tag{3.119}$$

which corresponds to the classical relations between velocity and linear momentum. Since these operators equations are of the same form as the classical equation, it is ensured that the quantum mechanical expectation values satisfy the classical equations of motion. In relativistic quantum theory, the situation is different. E.g., the expression for the "velocity operator" of a relativistic spin-0 particle was given by

$$\frac{d\vec{x}}{dt} = \frac{1}{i\hbar}\,[\hat{x}_1,\hat{H}_f] = (\hat{\tau}_3 + i\tau_2)\,\frac{\hat{p}}{m}\ , \tag{3.120}$$

while the classical relativistic velocity is given by

$$\frac{dx}{dt} = \frac{p}{M} = \frac{c^2 p}{Mc^2} = \frac{c^2 p}{E}\ , \tag{3.121}$$

where $M = \frac{m}{(1-\frac{v^2}{c^2})^{1/2}}$ denotes the relativistic mass, i.e.,

$$\begin{aligned} E = Mc^2 &= \frac{mc^2}{\sqrt{1 - \frac{v^2}{c^2}}} = \frac{mc^2}{\sqrt{1 - \frac{v^2}{c^2}}}\sqrt{\frac{v^2}{c^2} + \left(1 - \frac{v^2}{c^2}\right)} \\ &= c\sqrt{\frac{m^2v^2 + m^2c^2\,(1 - \frac{v^2}{c^2})}{1 - \frac{v^2}{c^2}}} \\ &= c\sqrt{\left(\frac{mv}{(1 - \frac{v^2}{c^2})^{1/2}}\right)^2 + m^2c^2} = c\sqrt{p^2 + m^2c^2} \end{aligned} \tag{3.122}$$

is the total energy of a free particle with rest mass $m$. Obviously, the right-hand side of (3.120) is different from the left-hand side. Furthermore, the eigenvalues of the matrix

$$\hat{\tau}_3 + i\hat{\tau}_2 = \begin{pmatrix} 1 & 1 \\ -1 & -1 \end{pmatrix} \tag{3.123}$$

are zero. This means that the eigenvalues of the velocity operator (3.120) are also zero. Hence, we again notice that, in general within a relativistic theory, the expectation values of a reasonably constructed operator are **not** the same as the values of the corresponding classical quantity. Thus, we conclude that not all operators of the non-relativistic theory can be transferred to a relativistic one-particle theory. The reason for this is the *restriction to the one-particle concept*. In relativistic quantum mechanics, the consistency of the one-particle description is limited. To be mathematically precise, the formulation of the relativistic theory within a one-particle concept implies the condition that the only valid operators are those which do not mix different charge states. Such operators are called **even operators** or **true one-particle operators**.

More formally, an operator $\hat{O}_{even}$ is called **even** if

$$\hat{O}_{even}\ \Psi^{\pm} \ = \ \Psi'^{(\pm)}\ , \tag{3.124}$$

where $\Psi'^{(\pm)}$ are functions with positive and negative frequencies. Similarly, an operator $\hat{O}_{odd}\ \Psi^(\pm)$ is called **odd** if

$$\hat{O}_{odd}\ \Psi^{(\pm)} \ = \ \Psi''^{(\mp)}\ . \tag{3.125}$$

Thus, the Hamiltonian of the free Klein-Gordon equation in the Schrödinger representation, $\hat{H}_f$, and the momentum operator $\hat{p} = -i\hbar\vec{\nabla}$ are even operators.

In general, an operator can be split into an even and odd part

$$\hat{O} \ = \ \hat{O}_{even} \ + \ \hat{O}_{odd}\ , \tag{3.126}$$

thus, one can separate from any given operator $\hat{O}$ a true one-particle operator $\hat{O}_{even}$. In matrix notation

$$\hat{O} \ = \ \begin{pmatrix} \hat{a}_{11} & 0 \\ 0 & \hat{a}_{22} \end{pmatrix} \ + \ \begin{pmatrix} 0 & \hat{a}_{12} \\ \hat{a}_{21} & 0 \end{pmatrix} \ = \ \hat{O}_{even} \ + \ \hat{O}_{odd}\ . \tag{3.127}$$

## 3.8 Klein-Gordon Equation with Interaction

To introduce electromagnetic interactions into the KG equation, we use the socalled 'minimal substitution', known from EM

$$p^\mu \to p^\mu - eA^\mu \tag{3.128}$$

where $A^\mu$ is a four-vector potential. Inserting this into the KG equation (3.15) gives

$$\left[-\left(i\frac{\partial}{\partial x^\mu} - eA_\mu\right)\left(i\frac{\partial}{\partial x_\mu} - eA^\mu\right) + m^2\right]\Psi(x) = 0 \tag{3.129}$$

or

$$\left[\partial_\mu \partial^\mu + m^2 + U(x)\right]\Psi(x) = 0, \tag{3.130}$$

where the generalized potential $U(x)$ consists of a scalar and vector part

$$\begin{aligned} U(x) &= ie\frac{\partial}{\partial x^\mu}A^\mu + ieA^\mu\frac{\partial}{\partial x^\mu} - e^2 A^\mu A_\mu \\ &= i\frac{\partial}{\partial x^\mu}V^\mu + iV^\mu\frac{\partial}{\partial x^\mu} + S \end{aligned} \tag{3.131}$$

Note that the symmetrized from of the vector terms is required in order to maintain the hermicity of the interaction. In the most general case, the scalar, $S$, and vector, $V^\mu$, parts of the potential can be independent interactions. For the electromagnetic case they are related by

$$\begin{aligned} S &= e^2 A^\mu A_\mu \\ V^\mu &= eA^\mu \end{aligned} \tag{3.132}$$

Using the 'standard' form of $A^\mu \equiv (\Phi, \mathbf{A})$, the KG equation can be written as

$$\left(i\frac{\partial}{\partial t} - e\Phi\right)^2 \Psi(\mathbf{x}, t) = \left[(-i\nabla - e\mathbf{A}^2)^2 + m^2\right]\Psi(\mathbf{x}, t) \tag{3.133}$$

Substituting the positive and negative energy solutions (3.23) into (3.133) gives

$$(E_p \mp e\Phi)^2 \Psi^{(\pm)}(\mathbf{x}, t) = \left[(\hat{p} \mp e\mathbf{A})^2 + m^2\right]\Psi^{(\pm)}(\mathbf{x}, t) \tag{3.134}$$

Again, once can use (3.134) as starting point and use it with more general potentials $V$ and $\mathbf{A}$. For example, let $\mathbf{A} = 0$ and $V = e\Phi$, i.e. allow only a scalar potential $V$. Then (3.134) gives

$$(E^2 + V^2 - 2EV)\Psi = (\hat{p}^2 + m^2)\Psi \tag{3.135}$$

Substituting the relation $E62 = k^2 + m^2$ between energy and wave vector and using $\hat{p} \to -i\nabla$ leads to

$$(\nabla^2 + k^2)\Psi = (2EV - V^2)\Psi, \tag{3.136}$$

which looks like a Schrödinger equation with the equivalent energy dependent potential

$$V^{SE} = \frac{2EV - V^2}{2m} \tag{3.137}$$

Another type of potential to consider is the Lorentz scalar, which adds to the mass, since $p^\mu p_\mu = m^2$. The KG equation with coupling to the scalar potential is

$$E^2\Psi = \left[\hat{p}^2 + (m+S)^2\right]\Psi \tag{3.138}$$