Chapter 7

Klein-Gordon Field

The first relativistic quantum field, which we deal with here, is the Klein-Gordon field. It represents a free scalar field and describes in its second-quantized form particles with spin 0. One example for such particles within the realm of the standard model of elementary particles is the Higgs particle H, which is electrically neutral and gives all particles their mass due to its interaction with them. Another example is provided by the pions, which were originally introduced by Hideki Yukawa as the exchange particles giving rise to the nuclear force. There exists a neutral pion π^0 and two charged pions with π^+ and its antiparticle π^-. Note that the pions turned out to be the lightest mesons, i.e. they consist of two quarks. Therefore, they are are unstable, decay via weak or electromagnetic interaction, and are considered nowadays no longer as elementary particles.

Coupling the charged pions minimally to the electromagnetic field yields a theory, which is called scalar electrodynamics. In its second quantized form it microscopically describes the interaction between charged pions due to the exchange of photons. From a pedagogical point of view it would be reasonable to introduce scalar QED before QED as the description of matter by the Klein-Gordon theory is much simpler than the Dirac theory. Therefore, starting with scalar QED would make it easier to understand several technical issues as, for instance, the Feynman diagrams of QED without having to deal with the intricate spinor algebra of the Dirac theory. Another motivation to study scalar electrodynamics would he that it represents the relativistic generalization of the Ginzburg-Landau theory of superconductivity. However, due to time constraints, we will not be able to work out scalar electrodynamics, so here we can only refer the interested reader to the relevant literature.

7.1 Action and Equations of Motions

The action of the Schrödinger fields $\psi(\mathbf{x}, t)$ and $\psi^*(\mathbf{x}, t)$ in (4.8)–(4.10) is not invariant with respect to Lorentz transformations as it contains partial derivatives of first (second) order with respect to the time (space) coordinate(s). In contrast to that a relativistic action must treat

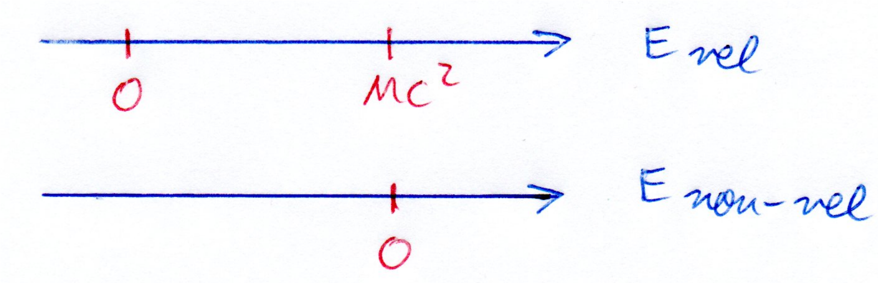

Figure 7.1: Comparison of relativistic and non-relativistic energy scales.

temporal and spatial partial derivatives on an equal footing. Depending on the respective internal spin degrees of freedom there are different ways how to convert the non-relativistic Schrödinger action (4.8)–(4.10) into a relativistic one.

In the following we deal with charged relativistic particles like the pions π^+ and π^-, which do not have any internal spin degree of freedom. Such particles are described by Klein-Gordon fields $\Psi(x^\lambda)$ and $\Psi^*(x^\lambda)$. The corresponding action

$$\mathcal{A} = \mathcal{A}\left[\Psi^*(\bullet); \Psi(\bullet)\right] \tag{7.1}$$

is defined by a spatio-temporal integral over the Lagrange density according to

$$\mathcal{A} = \frac{1}{c} \int d^4x \, \mathcal{L}\Big(\Psi^*(x^\lambda), \partial_\mu \Psi^*(x^\lambda); \Psi(x^\lambda), \partial_\nu \Psi(x^\lambda)\Big) \,, \tag{7.2}$$

where we have $d^4x = cdt\, d^3x$. The Lagrange density of the Klein-Gordon fields is given by the real-valued Lorentz invariant

$$\mathcal{L} = A \, g^{\mu\nu} \, \partial_\mu \Psi^*(x^\lambda) \, \partial_\nu \Psi(x^\lambda) + B \, \Psi^*(x^\lambda) \Psi(x^\lambda) \,. \tag{7.3}$$

In the following we choose the yet unknown constants A and B in such a way that the Lagrange density of the Klein-Gordon fields (7.3) goes over in the non-relativistic limit into the Lagrange density (4.10) of the Schrödinger fields. To this end we decompose at first the derivatives in (7.3) into their respective temporal and spatial contributions:

$$\mathcal{L} = A \left\{ \frac{1}{c^2} \frac{\partial \Psi^*(\mathbf{x},t)}{\partial t} \frac{\partial \Psi(\mathbf{x},t)}{\partial t} - \boldsymbol{\nabla} \, \Psi^*(\mathbf{x},t) \, \boldsymbol{\nabla} \Psi(\mathbf{x},t) \right\} + B \, \Psi^*(\mathbf{x},t) \, \Psi(\mathbf{x},t) \,. \tag{7.4}$$

Performing the transition from a relativistic to the corresponding non-relativistic theory one has to take into account that the corresponding energy scales are shifted by the rest energy Mc^2 of the particles with mass M with respect to each other:

$$E_{\rm rel} = E_{\rm non-rel} + Mc^2 \,. \tag{7.5}$$

This becomes apparent from Fig. 6.1, where the relativistic dispersion relation is compared with its non-relativistic limit, and is illustrated in Fig. 7.1. As a quantum mechanical wave function depends exponentially via $e^{-iEt/\hbar}$ from the energy E, (7.5) suggests to perform the separation ansatz

$$\Psi(\mathbf{x},t) = e^{-iMc^2t/\hbar}\,\psi(\mathbf{x},t)\,, \tag{7.6}$$

$$\Psi^*(\mathbf{x},t) = e^{iMc^2t/\hbar}\,\psi^*(\mathbf{x},t)\,. \tag{7.7}$$

Inserting (7.6), (7.7) into the Lagrange density of the Klein-Gordon fields (7.3), we obtain

$$\begin{aligned}\mathcal{L} &= \frac{A}{c^2}\left\{\frac{\partial\psi^*(\mathbf{x},t)}{\partial t}\,\frac{\partial\psi(\mathbf{x},t)}{\partial t} + \frac{i}{\hbar}\,Mc^2\left[\psi^*(\mathbf{x},t)\,\frac{\partial\psi(\mathbf{x},t)}{\partial t} - \frac{\partial\psi^*(\mathbf{x},t)}{\partial t}\,\psi(\mathbf{x},t)\right]\right\}\\ &\quad -A\,\boldsymbol{\nabla}\psi^*(\mathbf{x},t)\,\boldsymbol{\nabla}\psi(\mathbf{x},t) + \left(B + \frac{M^2c^2}{\hbar^2}\,A\right)\,\psi^*(\mathbf{x},t)\,\psi(\mathbf{x},t)\,.\end{aligned} \tag{7.8}$$

In the non-relativistic limit $c \to \infty$ we have now to guarantee that (7.8) reduces term by term to (4.10):

- Due to a partial integration in time the second and third term in (7.8) can be merged. A comparison with (4.10) then fixes the constant A:

$$\frac{2Mi}{\hbar}\,A = i\hbar \qquad \Longrightarrow \qquad A = \frac{\hbar^2}{2M}\,. \tag{7.9}$$

- With this choice of A the first term in (7.8) vanishes in the non-relativistic limit $c \to \infty$ and the fourth term turns out to yield the correct kinetic energy of the Schrödinger field.

- The last term in (7.8) must vanish as the Schrödinger field does not have such a mass term, so also the constant B is determined by taking into account (7.9)

$$B = -\frac{M^2c^2}{\hbar^2}\,A \qquad \Longrightarrow \qquad B = -\frac{1}{2}\,Mc^2\,. \tag{7.10}$$

Inserting (7.9) and (7.10) into (7.4) the action of the Klein-Gordon field

$$\mathcal{A} = \mathcal{A}\left[\Psi^*(\bullet,\bullet);\Psi(\bullet,\bullet)\right] \tag{7.11}$$

is given by a spatio-temporal integral

$$\mathcal{A} = \int dt \int d^3x\,\mathcal{L}\Big(\Psi^*(\mathbf{x},t),\,\boldsymbol{\nabla}\Psi^*(\mathbf{x},t),\,\frac{\partial\Psi^*(\mathbf{x},t),}{\partial t};\Psi(\mathbf{x},t),\,\boldsymbol{\nabla}\Psi(\mathbf{x},t),\,\frac{\partial\Psi(\mathbf{x},t),}{\partial t}\Big) \tag{7.12}$$

with the Lagrange density

$$\mathcal{L} = \frac{\hbar^2}{2Mc^2}\,\frac{\partial\Psi^*(\mathbf{x},t)}{\partial t}\,\frac{\partial\Psi(\mathbf{x},t)}{\partial t} - \frac{\hbar^2}{2M}\,\boldsymbol{\nabla}\,\Psi^*(\mathbf{x},t)\,\boldsymbol{\nabla}\Psi(\mathbf{x},t) - \frac{Mc^2}{2}\,\Psi^*(\mathbf{x},t)\,\Psi(\mathbf{x},t)\,. \tag{7.13}$$

Similar to the discussion of the Schrödinger fields in Section 4.4 the Hamilton principle of classical field theory

$$\frac{\delta\mathcal{A}}{\delta\Psi^*(\mathbf{x},t)} = 0\,, \qquad \Longrightarrow \qquad \frac{\delta\mathcal{A}}{\delta\Psi(\mathbf{x},t)} = 0 \tag{7.14}$$

leads to the Euler-Lagrange equations

$$\frac{\partial \mathcal{L}}{\partial \Psi^*(\mathbf{x},t)} - \boldsymbol{\nabla}\,\frac{\partial \mathcal{L}}{\partial \boldsymbol{\nabla}\Psi^*(\mathbf{x},t)} - \frac{\partial}{\partial t}\,\frac{\partial \mathcal{L}}{\partial \frac{\Psi^*(\mathbf{x},t)}{\partial t}} = 0\,, \tag{7.15}$$

$$\frac{\partial \mathcal{L}}{\partial \Psi(\mathbf{x},t)} - \boldsymbol{\nabla}\,\frac{\partial \mathcal{L}}{\partial \boldsymbol{\nabla}\Psi(\mathbf{x},t)} - \frac{\partial}{\partial t}\,\frac{\partial \mathcal{L}}{\partial \frac{\Psi(\mathbf{x},t)}{\partial t}} = 0\,. \tag{7.16}$$

In order to evaluate (7.15), (7.16) we need the following partial derivatives from the Lagrange density (7.13):

$$\frac{\partial \mathcal{L}}{\partial \Psi^*(\mathbf{x},t)} = -\frac{1}{2}\,Mc^2\Psi(\mathbf{x},t)\,, \frac{\partial \mathcal{L}}{\partial \boldsymbol{\nabla}\Psi^*(\mathbf{x},t)} = -\frac{\hbar^2}{2M}\,\boldsymbol{\nabla}\Psi(\mathbf{x},t)\,, \frac{\partial \mathcal{L}}{\partial \frac{\Psi^*(\mathbf{x},t)}{\partial t}} = \frac{\hbar^2}{2Mc^2}\,\frac{\Psi(\mathbf{x},t)}{\partial t}\,, \tag{7.17}$$

$$\frac{\partial \mathcal{L}}{\partial \Psi(\mathbf{x},t)} = -\frac{1}{2}\,Mc^2\Psi^*(\mathbf{x},t)\,, \frac{\partial \mathcal{L}}{\partial \boldsymbol{\nabla}\Psi(\mathbf{x},t)} = -\frac{\hbar^2}{2M}\,\boldsymbol{\nabla}\Psi^*(\mathbf{x},t)\,, \frac{\partial \mathcal{L}}{\partial \frac{\Psi(\mathbf{x},t)}{\partial t}} = \frac{\hbar^2}{2Mc^2}\,\frac{\Psi^*(\mathbf{x},t)}{\partial t}\,. \tag{7.18}$$

Inserting the additional calculation (7.17) and (7.18) into the Euler-Lagrange equations (7.15), (7.16), we obtain the Klein-Gordon equations for the fields $\Psi(\mathbf{x},t)$ and $\Psi^*(\mathbf{x},t)$:

$$\frac{1}{c^2}\,\frac{\partial^2\Psi(\mathbf{x},t)}{\partial t^2} - \boldsymbol{\nabla}^2\Psi(\mathbf{x},t) + \frac{M^2c^2}{\hbar^2}\,\Psi(\mathbf{x},t) = 0\,, \tag{7.19}$$

$$\frac{1}{c^2}\,\frac{\partial^2\Psi^*(\mathbf{x},t)}{\partial t^2} - \boldsymbol{\nabla}^2\Psi^*(\mathbf{x},t) + \frac{M^2c^2}{\hbar^2}\,\Psi^*(\mathbf{x},t) = 0\,. \tag{7.20}$$

They represent wave equations, which contain an additional term due to the finiteness of the Compton wave length of the particles

$$\lambda_{\mathrm{C}} = 2\pi\,\frac{\hbar}{Mc}\,. \tag{7.21}$$

For a pion π^+ or π^- with the rest energy $Mc^2 = 139.6$ MeV the Compton wave length (7.21) amounts to $\lambda_{\mathrm{C}} \approx 9$ fm, which is of the order of magnitude of the size of the atomic nucleus.

The appearance of the Compton wave length (7.21) can be physically understood as follows. A relativistic particle with the momentum uncertainty $\Delta p = Mc$ yields via the Heisenberg uncertainty relation a corresponding spatial uncertainty

$$\Delta x = \frac{\hbar}{Mc}\,, \tag{7.22}$$

which is of the order of the Compton wave length (7.21). Wherever a relativistic particle is confined to a region, which is of the order of the Compton wave length, the resulting energy uncertainty becomes so large that particle-antiparticle pairs are generated out of the vacuum. This peculiar phenomenon is best illustrated by the Klein paradox, which arises for a pion π^+ running against a potential step of height V, see Fig. 7.2. Provided that the potential height V reaches the order of the rest energy $2Mc^2$ of two pions, the wave function falls off exponentially in the region of the potential threshold. This then leads to the generation of particle-antiparticle pairs, which have to move due to momentum conservation in opposite directions. As a consequence, one observes within the potential threshold a negative charge

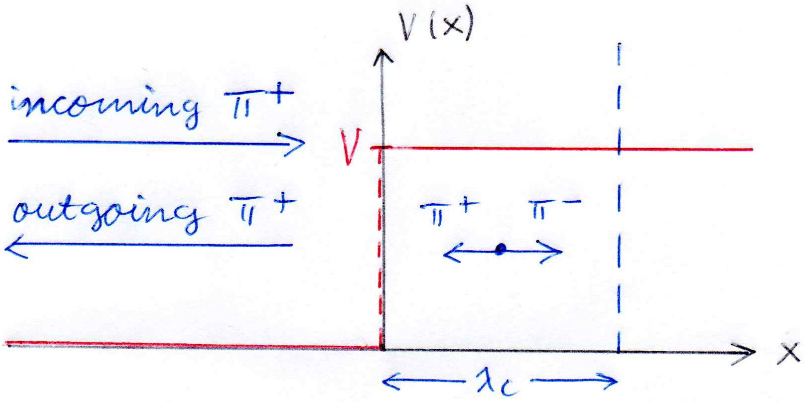

Figure 7.2: The scattering of a pion π^+ at a potential threshold with height $V \sim 2Mc^2$ leads to the Klein paradox that the reflection coefficient becomes larger than one. This is due to the creation of particle-antiparticle pairs within a region, which has the extension of the Compton wave length (7.22).

density, so that the situation emerges as depicted in Fig. 7.2. Surprisingly, this leads to a reflection coefficient of this one-particle scattering problem, which is larger than one. The Klein paradox has, therefore, the consequence that a relativistic quantum theory can never be restricted to a one-particle theory. Instead, it has to be extended to a relativistic quantum field theory in order to incorporate adequately the inherent many-body phenomena. Inserting the ansatz (7.6), (7.7) in the Klein-Gordon equations (7.19), (7.20) for the wave functions $\Psi(\mathbf{x}, t)$, $\Psi^*(\mathbf{x}, t)$, we obtain

$$\frac{1}{c^2}\frac{\partial^2\psi(\mathbf{x},t)}{\partial t^2} - \frac{2iM}{\hbar}\frac{\partial\psi(\mathbf{x},t)}{\partial t} - \boldsymbol{\nabla}^2\psi(\mathbf{x},t) = 0\,, \tag{7.23}$$

$$\frac{1}{c^2}\frac{\partial^2\psi^*(\mathbf{x},t)}{\partial t^2} + \frac{2iM}{\hbar}\frac{\partial\psi^*(\mathbf{x},t)}{\partial t} - \boldsymbol{\nabla}^2\psi^*(\mathbf{x},t) = 0\,. \tag{7.24}$$

In the non-relativistic limit $c \to \infty$ both (7.23) and (7.24) go over into the corresponding Schrödinger equations for the wave functions $\psi(\mathbf{x}, t)$ and $\psi^*(\mathbf{x}, t)$, as expected:

$$i\hbar\frac{\partial\Psi(\mathbf{x},t)}{\partial t} = -\frac{\hbar^2}{2M}\boldsymbol{\nabla}^2\Psi(\mathbf{x},t)\,, \tag{7.25}$$

$$-i\hbar\frac{\partial\Psi^*(\mathbf{x},t)}{\partial t} = -\frac{\hbar^2}{2M}\boldsymbol{\nabla}^2\,\Psi^*(\mathbf{x},t)\,. \tag{7.26}$$

Note that, historically, Erwin Schrödinger discovered on his quest for a quantum mechanical wave equation in 1926 at first the Klein-Gordon equation. But solving this relativistic wave equation for the example of the Coulomb potential he found that the resulting energy eigenvalues disagreed with the measured spectral lines of the hydrogen atom. In retrospect we know that this is due to the fact that the Klein-Gordon equation does not take into account the spin 1/2 degree of freedom of the electron in the hydrogen atom. Due to this discrepancy he abandoned the Klein-Gordon equation and derived instead in the non-relativistic limit the

Schrödinger equation, where he obtained a much better agreement between the corresponding solution of the Coulomb problem and the measured spectral lines of the hydrogen atom.

7.2 Continuity Equation

Now we multiply (7.19) with $\Psi^*(\mathbf{x},t)$ and (7.20) with $\Psi(\mathbf{x},t)$ and subtract both from each other, yielding at first

$$\frac{1}{c^2}\Psi^*(\mathbf{x},t)\frac{\partial^2\Psi(\mathbf{x},t)}{\partial t^2}-\frac{1}{c^2}\Psi(\mathbf{x},t)\frac{\partial^2\Psi^*(\mathbf{x},t)}{\partial t^2}-\Psi^*(\mathbf{x},t)\boldsymbol{\nabla}^2\Psi(\mathbf{x},t)+\Psi(\mathbf{x},t)\boldsymbol{\nabla}^2\Psi^*(\mathbf{x},t)=0\,, \tag{7.27}$$

where the mass terms have dropped out. This can be recast into the form

$$\begin{aligned}\frac{\partial}{\partial t}\left\{\Psi^*(\mathbf{x},t)\,\frac{\partial\Psi(\mathbf{x},t)}{\partial t}-\frac{\partial\Psi^*(\mathbf{x},t)}{\partial t}\,\Psi(\mathbf{x},t)\right\}&\\ +\boldsymbol{\nabla}\Big\{\Psi(\mathbf{x},t)\,\boldsymbol{\nabla}\Psi^*(\mathbf{x},t)-\Psi^*(\mathbf{x},t)\,\boldsymbol{\nabla}\Psi(\mathbf{x},t)\Big\}&=0\,.\end{aligned} \tag{7.28}$$

which corresponds to a continuity equation:

$$\frac{\partial\rho(\mathbf{x},t)}{\partial t}+\boldsymbol{\nabla}\mathbf{j}(\mathbf{x},t)=0\,. \tag{7.29}$$

Here both density $\rho(\mathbf{x},t)$ and current density $\mathbf{j}(\mathbf{x},t)$ are only determined up to a yet unknown constant K:

$$\rho(\mathbf{x},t) = \frac{K}{c^2}\left\{\Psi^*(\mathbf{x},t)\,\frac{\partial\Psi(\mathbf{x},t)}{\partial t}-\frac{\partial\Psi^*(\mathbf{x},t)}{\partial t}\,\Psi(\mathbf{x},t)\right\}, \tag{7.30}$$

$$\mathbf{j}(\mathbf{x},t) = K\Big\{\Psi(\mathbf{x},t)\,\boldsymbol{\nabla}\Psi^*(\mathbf{x},t)-\Psi^*(\mathbf{x},t)\,\boldsymbol{\nabla}\Psi(\mathbf{x},t)\Big\}. \tag{7.31}$$

The constant K can now be fixed uniquely by considering the non-relativistic limit $c\to\infty$. To this end one inserts the ansatz (7.19), (7.20) into (7.30), (7.31) and gets

$$\rho(\mathbf{x},t) = \frac{K}{c^2}\left\{\psi^*(\mathbf{x},t)\,\frac{\partial\psi(\mathbf{x},t)}{\partial t}-\frac{\partial\psi^*(\mathbf{x},t)}{\partial t}\,\psi(\mathbf{x},t)-\frac{2iMc^2}{\hbar}\,\psi^*(\mathbf{x},t)\psi(\mathbf{x},t)\right\}, \tag{7.32}$$

$$\mathbf{j}(\mathbf{x},t) = K\Big\{\psi(\mathbf{x},t)\,\boldsymbol{\nabla}\Psi^*(\mathbf{x},t)-\psi^*(\mathbf{x},t)\,\boldsymbol{\nabla}\psi(\mathbf{x},t)\Big\}. \tag{7.33}$$

We have then to demand that (7.32), (7.33) go over in the non-relativistic limit $c\to\infty$ to the corresponding non-relativistic expressions:

$$\rho(\mathbf{x},t) = \psi^*(\mathbf{x},t)\psi(\mathbf{x},t)\,, \tag{7.34}$$

$$\mathbf{j}(\mathbf{x},t) = \frac{i\hbar}{2M}\Big\{\psi(\mathbf{x},t)\,\boldsymbol{\nabla}\psi^*(\mathbf{x},t)-\psi^*(\mathbf{x},t)\,\boldsymbol{\nabla}\psi(\mathbf{x},t)\Big\}. \tag{7.35}$$

This fixes the constant K to the value

$$K=\frac{i\hbar}{2M}\,. \tag{7.36}$$

Thus, we obtain from (7.30), (7.31), and (7.36) for the density $\rho(\mathbf{x},t)$ and the current density $\mathbf{j}(\mathbf{x},t)$ of the Klein-Gordon fields

$$\rho(\mathbf{x},t) = \frac{i\hbar}{2Mc^2}\left\{\Psi^*(\mathbf{x},t)\,\frac{\partial\Psi(\mathbf{x},t)}{\partial t} - \frac{\partial\Psi^*(\mathbf{x},t)}{\partial t}\,\Psi(\mathbf{x},t)\right\}, \tag{7.37}$$

$$\mathbf{j}(\mathbf{x},t) = \frac{i\hbar}{2M}\left\{\Psi(\mathbf{x},t)\,\boldsymbol{\nabla}\Psi^*(\mathbf{x},t) - \Psi^*(\mathbf{x},t)\,\boldsymbol{\nabla}\Psi(\mathbf{x},t)\right\}. \tag{7.38}$$

From the continuity equation (7.29) follows the existence of the conserved quantity. Namely, considering the time derivative of the quantity

$$Q = \int d^3x\,\rho(\mathbf{x},t)\,, \tag{7.39}$$

we obtain from (7.29) and applying the theorem of Gauß

$$\frac{\partial Q}{\partial t} = -\oint d\mathbf{f}\cdot\mathbf{j}(\mathbf{x},t)\,. \tag{7.40}$$

Here the surface integral at infinity vanishes as the fields $\Psi^*(\mathbf{x},t)$, $\Psi(\mathbf{x},t)$ as well as the current density $\mathbf{j}(\mathbf{x},t)$ in (7.38) are assumed to vanish fast enough at infinity, yielding

$$\frac{\partial Q}{\partial t} = 0\,. \tag{7.41}$$

Now it turns out to be useful to define a scalar product between two arbitrary fields $\Psi_1(\mathbf{x},t)$ and $\Psi_2(\mathbf{x},t)$ according to

$$\langle\Psi_1,\Psi_2\rangle = \frac{i\hbar}{2Mc^2}\int d^3x\left\{\Psi_1^*(\mathbf{x},t)\,\frac{\partial\Psi_2(\mathbf{x},t)}{\partial t} - \frac{\partial\Psi_1^*(\mathbf{x},t)}{\partial t}\,\Psi_2(\mathbf{x},t)\right\}. \tag{7.42}$$

But note that this scalar product is not positive definite. For instance, choosing the ansatz

$$\Psi_1(\mathbf{x},t) = \Psi_2(\mathbf{x},t) = N\,e^{iMc^2t/\hbar} \tag{7.43}$$

we obtain

$$\langle\Psi_1,\Psi_2\rangle = -N^2 < 0\,. \tag{7.44}$$

In order to investigate the non-relativistic limit of this scalar product, we insert (7.6), (7.7) into (7.42):

$$\langle\Psi_1,\Psi_2\rangle = \frac{i\hbar}{2Mc^2}\int d^3x\left\{\psi_1^*(\mathbf{x},t)\frac{\partial\psi_2(\mathbf{x},t)}{\partial t} - \frac{\partial\psi_1(\mathbf{x},t)}{\partial t}\psi_2(\mathbf{x},t) - \frac{2iMc^2}{\hbar}\psi_1^*(\mathbf{x},t)\psi_2(\mathbf{x},t)\right\} \tag{7.45}$$

Performing the limit $c\to\infty$, we conclude

$$\langle\Psi_1,\Psi_2\rangle = \lim_{c\to\infty}\langle\Psi_1,\Psi_2\rangle = \int d^3x\,\psi_1^*(\mathbf{x},t)\psi_2(\mathbf{x},t)\,, \tag{7.46}$$

which is just the positive definite scalar product used in the Schrödinger theory. Thus, from the fact, that the scalar products of the Klein-Gordon and the Schrödinger theory differ, we read off that each quantum field theory has its own natural scalar product. It turns out that this conclusion has far-reaching consequences, as the natural scalar product of a quantum field theory represents a central technical tool. For instance, in the present case of the Klein-Gordon theory, taking into account (7.37) we finally obtain a useful relation between the conserved quantity (7.42) and the scalar product (7.39):

$$Q = \langle \Psi, \Psi \rangle \,. \tag{7.47}$$

As the scalar product is not positive definite, the conserved quantity can have both positive and negative values. This makes it possible to identify Q, or more precisely eQ with the electric charge of a complex-valued Klein-Gordon field, where e denotes the elementary charge. Furthermore, we conclude that a real-valued Klein-Gordon field, where $\Psi^*(\mathbf{x}, t) = \Psi(\mathbf{x}, t)$ holds, leads to a vanishing charge Q due to (7.42) and (7.47).

7.3 Canonical Field Quantization

The two independent Klein-Gordon fields $\Psi^*(\mathbf{x}, t)$ and $\Psi(\mathbf{x}, t)$ have the two following two canonically conjugated momentum fields:

$$\Pi^*(\mathbf{x}, t) = \frac{\partial \mathcal{L}}{\frac{\partial \Psi^*(\mathbf{x},t)}{\partial t}} = \frac{\hbar^2}{2Mc^2} \, \frac{\partial \Psi(\mathbf{x}, t)}{\partial t} \,, \tag{7.48}$$

$$\Pi(\mathbf{x}, t) = \frac{\partial \mathcal{L}}{\frac{\partial \Psi(\mathbf{x},t)}{\partial t}} = \frac{\hbar^2}{2Mc^2} \, \frac{\partial \Psi^*(\mathbf{x}, t)}{\partial t} \,. \tag{7.49}$$

where $\mathcal{L}$ denotes the Lagrange density of the Klein-Gordon field from (7.13). With the help of a Legendre transformation we then obtain the Hamilton density from the Lagrange density:

$$\mathcal{H} = \Pi^*(\mathbf{x}, t) \, \frac{\partial \Psi^*(\mathbf{x}, t)}{\partial t} + \Pi(\mathbf{x}, t) \, \frac{\partial \Psi(\mathbf{x}, t)}{\partial t} - \mathcal{L} \,. \tag{7.50}$$

Inserting therein (7.13) together with (7.48), (7.49) this yields

$$\mathcal{H} = \frac{2Mc^2}{\hbar^2} \, \Pi^*(\mathbf{x}, t)\Pi(\mathbf{x}, t) + \frac{\hbar^2}{2M} \, \boldsymbol{\nabla}\Psi^*(\mathbf{x}, t)\boldsymbol{\nabla}\Psi(\mathbf{x}, t) + \frac{Mc^2}{2} \, \Psi^*(\mathbf{x}, t)\Psi(\mathbf{x}, t) \,. \tag{7.51}$$

The Hamilton function H of the charged Klein-Gordon field then follows from spatially integrating this Hamilton density $\mathcal{H}$:

$$H = \int d^3x \, \mathcal{H} \,. \tag{7.52}$$

With this one can perform a canonical field quantization along the lines outlined in Chapter 5. For the sake of brevity we do not work this out in detail for the Klein-Gordon field but mention instead the result. At first, one assigns to the classical fields $\Psi^*(\mathbf{x}, t)$, $\Psi(\mathbf{x}, t)$, $\Pi^*(\mathbf{x}, t)$, and $\Pi(\mathbf{x},t)$ corresponding second-quantized operators $\hat{\Psi}^\dagger(\mathbf{x},t)$, $\hat{\Psi}(\mathbf{x},t)$, $\hat{\Pi}^\dagger(\mathbf{x},t)$, and $\hat{\Pi}(\mathbf{x},t)$. Due to the spin-statistic theorem of Pauli one performs for the Klein-Gordon field a bosonic field quantization and obtains between both $\hat{\Psi}(\mathbf{x},t)$, $\hat{\Pi}(\mathbf{x},t)$ and $\hat{\Psi}^\dagger(\mathbf{x},t)$, $\hat{\Pi}^\dagger(\mathbf{x},t)$ equal-time canonical commutation relations:

$$\left[\hat{\Psi}(\mathbf{x},t),\hat{\Psi}(\mathbf{x}',t)\right]=\left[\hat{\Pi}(\mathbf{x},t),\hat{\Pi}(\mathbf{x}',t)\right]=0, \quad \left[\hat{\Psi}(\mathbf{x},t),\hat{\Pi}(\mathbf{x}',t)\right]=i\hbar\,\delta(\mathbf{x}-\mathbf{x}')\,, \tag{7.53}$$

$$\left[\hat{\Psi}^\dagger(\mathbf{x},t),\hat{\Psi}^\dagger(\mathbf{x}',t)\right]=\left[\hat{\Pi}^\dagger(\mathbf{x},t),\hat{\Pi}^\dagger(\mathbf{x}',t)\right]=0, \quad \left[\hat{\Psi}^\dagger(\mathbf{x},t),\hat{\Pi}^\dagger(\mathbf{x}',t)\right]=i\hbar\,\delta(\mathbf{x}-\mathbf{x}')\,. \tag{7.54}$$

Due to the independence of the quantized degrees of freedom all mixed equal-time commutator relations vanish:

$$\left[\hat{\Psi}(\mathbf{x},t),\hat{\Psi}^\dagger(\mathbf{x}',t)\right]=\left[\hat{\Psi}(\mathbf{x},t),\hat{\Pi}^\dagger(\mathbf{x}',t)\right]=\left[\hat{\Pi}(\mathbf{x},t),\hat{\Psi}^\dagger(\mathbf{x}',t)\right]=\left[\hat{\Pi}(\mathbf{x},t),\hat{\Pi}^\dagger(\mathbf{x}',t)\right]=0\,. \tag{7.55}$$

Furthermore, the canonical field quantization converts the classical Hamilton function (7.51), (7.52) to the Hamilton operator:

$$\hat{H}=\int d^3x\left\{\frac{2Mc^2}{\hbar^2}\,\hat{\Pi}^\dagger(\mathbf{x},t)\hat{\Pi}(\mathbf{x},\mathbf{t})+\frac{\hbar^2}{2M}\,\boldsymbol{\nabla}\hat{\Psi}^\dagger(\mathbf{x},t)\boldsymbol{\nabla}\hat{\Psi}(\mathbf{x},t)+\frac{Mc^2}{2}\,\hat{\Psi}^\dagger(\mathbf{x},\mathbf{t})\hat{\Psi}(\mathbf{x},t)\right\}\,. \tag{7.56}$$

Note that the respective order of the operators in (7.56) does not play a role due to (7.55). With the Hamilton operator we then obtain the following Heisenberg equations:

$$i\hbar\,\frac{\partial\hat{\Psi}(\mathbf{x},t)}{\partial t}=\left[\hat{\Psi}(\mathbf{x},t),\hat{H}\right]_- \quad\Longrightarrow\quad \frac{\partial\hat{\Psi}(\mathbf{x},t)}{\partial t}=\frac{2Mc^2}{\hbar^2}\,\hat{\Pi}^\dagger(\mathbf{x},t)\,, \tag{7.57}$$

$$i\hbar\,\frac{\partial\hat{\Psi}^\dagger(\mathbf{x},t)}{\partial t}=\left[\hat{\Psi}^\dagger(\mathbf{x},t),\hat{H}\right]_- \quad\Longrightarrow\quad \frac{\partial\hat{\Psi}^\dagger(\mathbf{x},t)}{\partial t}=\frac{2Mc^2}{\hbar^2}\,\hat{\Pi}(\mathbf{x},t)\,, \tag{7.58}$$

$$i\hbar\,\frac{\partial\hat{\Pi}(\mathbf{x},t)}{\partial t}=\left[\hat{\Pi}(\mathbf{x},t),\hat{H}\right]_- \quad\Longrightarrow\quad \frac{\partial\hat{\Pi}(\mathbf{x},t)}{\partial t}=\frac{\hbar^2}{2M}\,\Delta\,\hat{\Psi}^\dagger(\mathbf{x},t)-\frac{Mc^2}{2}\,\hat{\Psi}^\dagger(\mathbf{x},t)\,, \tag{7.59}$$

$$i\hbar\,\frac{\partial\hat{\Pi}^\dagger(\mathbf{x},t)}{\partial t}=\left[\hat{\Pi}^\dagger(\mathbf{x},t),\hat{H}\right]_- \quad\Longrightarrow\quad \frac{\partial\hat{\Pi}^\dagger(\mathbf{x},t)}{\partial t}=\frac{\hbar^2}{2M}\,\Delta\,\hat{\Psi}(\mathbf{x},t)-\frac{Mc^2}{2}\,\hat{\Psi}(\mathbf{x},t)\,. \tag{7.60}$$

Note that the respective commutators are evaluated either with the operator identity (3.43) or with functional derivatives similar to Section 4.3. Furthermore, combining (7.57) and (7.60) as well as (7.58) and (7.59), we read off that both field operators $\hat{\Psi}^\dagger(\mathbf{x},t)$ and $\hat{\Psi}(\mathbf{x},t)$ obey the Klein-Gordon equation:

$$\left(\frac{1}{c^2}\frac{\partial}{\partial t^2}-\Delta+\frac{M^2c^2}{\hbar^2}\right)\hat{\Psi}(\mathbf{x},t)=0\,, \tag{7.61}$$

$$\left(\frac{1}{c^2}\frac{\partial}{\partial t^2}-\Delta+\frac{M^2c^2}{\hbar^2}\right)\hat{\Psi}^\dagger(\mathbf{x},t)=0\,. \tag{7.62}$$

In the following we determine the solutions of the operator-valued partial differential equations (7.61), (7.62) and work out their corresponding physical interpretation.

7.4 Plane Waves

The field operator $\hat{\Psi}(\mathbf{x}, t)$ as a function of its spatial degree of freedom $\mathbf{x}$ is now expanded into plane waves:

$$\hat{\Psi}(\mathbf{x}, t) = \int d^3p \, \hat{a}_{\mathbf{p}}(t) N_{\mathbf{p}} \exp\left\{\frac{i}{\hbar}\,\mathbf{p}\,\mathbf{x}\right\}. \tag{7.63}$$

Here $N_{\mathbf{p}}$ denotes a normalization constant, which is fixed later on appropriately. Inserting the decomposition (7.63) into the Klein-Gordon equation (7.61) of the field operator, yields an ordinary differential equation of second order for the respective Fourier operators $\hat{a}_{\mathbf{p}}(t)$:

$$\frac{\partial}{\partial t^2}\,\hat{a}_{\mathbf{p}}(t) + \frac{\mathbf{p}^2 c^2 + M^2 c^4}{\hbar^2}\,\hat{a}_{\mathbf{p}}(t) = 0\,. \tag{7.64}$$

The general solution of (7.64) reads

$$\hat{a}_{\mathbf{p}}(t) = \hat{a}_{\mathbf{p}}^{(1)} \exp\left\{-\frac{i}{\hbar}\,E_{\mathbf{p}} t\right\} + \hat{a}_{\mathbf{p}}^{(2)} \exp\left\{\frac{i}{\hbar}\,E_{\mathbf{p}} t\right\}. \tag{7.65}$$

Here we have introduced as an abbreviation the relativistic energy-momentum dispersion

$$E_{\mathbf{p}} = \sqrt{\mathbf{p}^2 c^2 + M^2 c^4}\,, \tag{7.66}$$

which obeys the symmetry

$$E_{\mathbf{p}} = E_{-\mathbf{p}}\,. \tag{7.67}$$

Inserting (7.65) into the plane wave expansion (7.63), we obtain at first

$$\hat{\Psi}(\mathbf{x}, t) = \int d^3p \, N_{\mathbf{p}} \left\{\hat{a}_{\mathbf{p}}^{(1)} \exp\left[\frac{i}{\hbar}\,(\mathbf{p}\mathbf{x} - E_{\mathbf{p}} t)\right] + \hat{a}_{\mathbf{p}}^{(2)} \exp\left[\frac{i}{\hbar}\,(\mathbf{p}\mathbf{x} + E_{\mathbf{p}} t)\right]\right\}. \tag{7.68}$$

Performing in the second term the substitution $\mathbf{p} \to -\mathbf{p}$, taking into account (7.67), and assuming

$$N_{\mathbf{p}} = N_{-\mathbf{p}} \tag{7.69}$$

converts (7.68) into

$$\hat{\Psi}(\mathbf{x}, t) = \int d^3p \, N_{\mathbf{p}} \left\{\hat{a}_{\mathbf{p}}^{(1)} \exp\left[\frac{i}{\hbar}\,(\mathbf{p}\mathbf{x} - E_{\mathbf{p}} t)\right] + \hat{a}_{-\mathbf{p}}^{(2)} \exp\left[-\frac{i}{\hbar}\,(\mathbf{p}\mathbf{x} - E_{\mathbf{p}} t)\right]\right\}. \tag{7.70}$$

Thus, redefining $\hat{a}_{-\mathbf{p}}^{(2)}$ as $\hat{a}_{\mathbf{p}}^{(2)}$ allows to compactly summarize (7.70) as

$$\hat{\Psi}(\mathbf{x}, t) = \sum_{r=1}^{2} \int d^3p \, \hat{a}_{\mathbf{p}}^{(r)}\, u_{\mathbf{p}}^{(r)}(\mathbf{x}, t)\,. \tag{7.71}$$

Here we have introduced $u_{\mathbf{p}}^{(r)}(\mathbf{x}, t)$ as an abbreviation for the plane waves

$$u_{\mathbf{p}}^{(r)}(\mathbf{x}, t) = N_{\mathbf{p}} \exp\left\{\varepsilon_r\,\frac{i}{\hbar}\,(\mathbf{p}\mathbf{x} - E_{\mathbf{p}} t)\right\} \tag{7.72}$$

with the notation

$$\varepsilon_r = \begin{cases} +1; & r = 1 \\ -1; & r = 2 \end{cases} . \tag{7.73}$$

The normalization constant $N_{\mathbf{p}}$ is now fixed by demanding for the scalar product between the plane waves $u_{\mathbf{p}}^{(r)}(\mathbf{x}, t)$ and $u_{\mathbf{p}'}^{(r')}(\mathbf{x}, t)$:

$$\langle u_{\mathbf{p}}^{(r)}, u_{\mathbf{p}'}^{(r')} \rangle = \varepsilon_r \, \delta_{r,r'} \, \delta(\mathbf{p} - \mathbf{p}') . \tag{7.74}$$

Thus, this condition amounts to demanding that the plane waves (7.72) with $r = 1$ and $r = 2$ correspond to the charge $+1$ and -1, respectively, as follows from (7.47) and (7.73). Taking into account the scalar product of the Klein-Gordon theory defined in (7.42) as well as (7.72), we get at first

$$\begin{aligned} \langle u_{\mathbf{p}}^{(r)}, u_{\mathbf{p}'}^{(r')} \rangle &= \frac{\varepsilon_r E_{\mathbf{p}} + \varepsilon_{r'} E_{\mathbf{p}'}}{2Mc^2} \, N_{\mathbf{p}} N_{\mathbf{p}'} \, \exp\left\{ \frac{i}{\hbar} \left(\varepsilon_r E_{\mathbf{p}} - \varepsilon_{r'} E_{\mathbf{p}'} \right) t \right\} \\ &\quad \times \int d^3x \, \exp\left\{ \frac{i}{\hbar} \left(\varepsilon_{r'} \mathbf{p}' - \varepsilon_r \mathbf{p} \right) \mathbf{x} \right\} . \end{aligned} \tag{7.75}$$

Performing the spatial integral yields $\delta(\varepsilon_{r'} \mathbf{p}' - \varepsilon_r \mathbf{p}) = \delta(\mathbf{p}' - \varepsilon_r \varepsilon_{r'} \mathbf{p})$, so we conclude from the symmetries (7.67) and (7.69):

$$\langle u_{\mathbf{p}}^{(r)}, u_{\mathbf{p}'}^{(r')} \rangle = \frac{(2\pi\hbar)^3 E_{\mathbf{p}}}{Mc^2} \, N_{\mathbf{p}}^2 \, \frac{\varepsilon_r + \varepsilon_{r'}}{2} \, \exp\left\{ \frac{i}{\hbar} \left(\varepsilon_r - \varepsilon_{r'} \right) E_{\mathbf{p}} t \right\} \delta(\mathbf{p}' - \varepsilon_r \varepsilon_{r'} \mathbf{p}) . \tag{7.76}$$

Due to the observation

$$\frac{\varepsilon_r + \varepsilon_{r'}}{2} = \begin{cases} \varepsilon_r; & r = r' \\ 0; & r \neq r' \end{cases} = \varepsilon_r \, \delta_{r,r'} \, , \tag{7.77}$$

which follows from (7.73), Eq. (7.76) reduces to (7.74) provided the normalization is fixed by

$$N_{\mathbf{p}} = \sqrt{\frac{Mc^2}{(2\pi\hbar)^3} \, E_{\mathbf{p}}} . \tag{7.78}$$

Indeed, the normalization (7.78) obeys the imposed symmetry (7.69) due to (7.67).

For the following calculations we need another technical result. Namely, considering the complex conjugated plane wave $u_{\mathbf{p}}^{(r)*}(\mathbf{x}, t)$, this just corresponds to exchanging the indices $r = 1$ and $r = 2$ according to (7.72):

$$u_{\mathbf{p}}^{(1)*}(\mathbf{x}, t) = u_{\mathbf{p}}^{(2)}(\mathbf{x}, t) , \qquad u_{\mathbf{p}}^{(2)*}(\mathbf{x}, t) = u_{\mathbf{p}}^{(1)}(\mathbf{x}, t) . \tag{7.79}$$

Therefore, we read off from (7.74) and (7.79) the scalar product between two complex conjugated plane waves:

$$\langle u_{\mathbf{p}}^{(r)*}, u_{\mathbf{p}'}^{(r')*} \rangle = -\varepsilon_r \, \delta_{r,r'} \, \delta(\mathbf{p} - \mathbf{p}') . \tag{7.80}$$

7.5 Fourier Operators

According to (7.71) and

$$\hat{\Psi}^\dagger(\mathbf{x},t) = \sum_{r=1}^{2} \int d^3p\, \hat{a}_{\mathbf{p}}^{(r)\dagger}\, u_{\mathbf{p}}^{(r)*}(\mathbf{x},t)\,. \tag{7.81}$$

both the field operator $\hat{\Psi}(\mathbf{x},t)$ and its adjoint $\hat{\Psi}^\dagger(\mathbf{x},t)$ are expanded in plane waves with time-independent Fourier operators $\hat{a}_{\mathbf{p}}^{(r)}$ and $\hat{a}_{\mathbf{p}}^{(r)\dagger}$. With the help of the scalar product of the Klein-Gordon field both relations can be inverted so that, conversely, the Fourier operators $\hat{a}_{\mathbf{p}}^{(r)}$ and $\hat{a}_{\mathbf{p}}^{(r)\dagger}$ are expressed in terms of the field operator $\hat{\Psi}(\mathbf{x},t)$ and its adjoint $\hat{\Psi}^\dagger(\mathbf{x},t)$. Taking into account (7.74) and (7.80) we get at first

$$\hat{a}_{\mathbf{p}}^{(r)} = \varepsilon_r \, \langle u_{\mathbf{p}}^{(r)}, \hat{\Psi} \rangle\,, \tag{7.82}$$

$$\hat{a}_{\mathbf{p}}^{(r)\dagger} = -\varepsilon_r \, \langle u_{\mathbf{p}}^{(r)*}, \hat{\Psi}^\dagger \rangle\,, \tag{7.83}$$

which reduces due to (7.42) to

$$\hat{a}_{\mathbf{p}}^{(r)} = \frac{i\hbar\varepsilon_r}{2Mc^2} \int d^3x \left\{ u^{(r)*}(\mathbf{x},t)\, \frac{\partial \hat{\Psi}(\mathbf{x},t)}{\partial t} - \frac{\partial u^{(r)*}(\mathbf{x},t)}{\partial t}\, \hat{\Psi}(\mathbf{x},t) \right\}, \tag{7.84}$$

$$\hat{a}_{\mathbf{p}}^{(r)\dagger} = \frac{-i\hbar\varepsilon_r}{2Mc^2} \int d^3x \left\{ u^{(r)}(\mathbf{x},t)\, \frac{\partial \hat{\Psi}^\dagger(\mathbf{x},t)}{\partial t} - \frac{\partial u^{(r)}(\mathbf{x},t)}{\partial t}\, \hat{\Psi}^\dagger(\mathbf{x},t) \right\}. \tag{7.85}$$

Applying the Heisenberg equations of motion (7.57) and (7.58) we arrive at the following representation for the Fourier operators:

$$\hat{a}_{\mathbf{p}}^{(r)} = \frac{i\hbar\varepsilon_r}{2Mc^2} \int d^3x \left\{ \frac{2Mc^2}{\hbar^2}\, u^{(r)*}(\mathbf{x},t)\, \hat{\Pi}^\dagger(\mathbf{x},t) - \frac{\partial u^{(r)*}(\mathbf{x},t)}{\partial t}\, \hat{\Psi}(\mathbf{x},t) \right\}, \tag{7.86}$$

$$\hat{a}_{\mathbf{p}}^{(r)\dagger} = \frac{-i\hbar\varepsilon_r}{2Mc^2} \int d^3x \left\{ \frac{2Mc^2}{\hbar^2}\, u^{(r)}(\mathbf{x},t)\, \hat{\Pi}(\mathbf{x},t) - \frac{\partial u^{(r)}(\mathbf{x},t)}{\partial t}\, \hat{\Psi}^\dagger(\mathbf{x},t) \right\}. \tag{7.87}$$

With this and the canonical equal-time commutator relations between the field operators and the momentum operators (7.53)–(7.55) we determine the commutation relations between the Fourier operators $\hat{a}_{\mathbf{p}}^{(r)}$ and $\hat{a}_{\mathbf{p}}^{(r)\dagger}$. At first we get straight-forwardly the trivial commutators

$$\left[\hat{a}_{\mathbf{p}}^{(r)}, \hat{a}_{\mathbf{p}'}^{(r')}\right]_- = \left[\hat{a}_{\mathbf{p}}^{(r)\dagger}, \hat{a}_{\mathbf{p}'}^{(r')\dagger}\right]_- = 0\,. \tag{7.88}$$

And for the non-trivial commutator we obtain at first

$$\left[\hat{a}_{\mathbf{p}}^{(r)}, \hat{a}_{\mathbf{p}'}^{(r')\dagger}\right]_- = \varepsilon_r\varepsilon_{r'} \frac{i\hbar}{2Mc^2} \int d^3x \left\{ u_{\mathbf{p}}^{(r)}(\mathbf{x},t)\, \frac{\partial u_{\mathbf{p}'}^{(r')}(\mathbf{x},t)}{\partial t} - \frac{\partial u_{\mathbf{p}}^{(r)}(\mathbf{x},t)}{\partial t}\, u_{\mathbf{p}'}^{(r')}(\mathbf{x},t) \right\}, \tag{7.89}$$

so taking into account (7.42), $\varepsilon_r^2 = 1$ due to (7.73), and (7.74) finally yields

$$\left[\hat{a}_{\mathbf{p}}^{(r)}, \hat{a}_{\mathbf{p}'}^{(r')\dagger}\right]_- = \varepsilon_r\, \delta_{r,r'}\, \delta(\mathbf{p}-\mathbf{p}')\,. \tag{7.90}$$

Here the appearance of the factor ε_r indicates due to (7.73) that $\hat{a}_{\mathbf{p}}^{(2)}$ and $\hat{a}_{\mathbf{p}}^{(2)\dagger}$ due not represent a creation and annihilation operator, respectively. We come back to this observation in due course, but before we determine how both the Hamilton operator and the charge operator are decomposed in terms of the Fourier operators $\hat{a}_{\mathbf{p}}^{(r)}$ and $\hat{a}_{\mathbf{p}}^{(r)\dagger}$.

7.6 Hamilton Operator

The plane wave expansions (7.71) and (7.81) of the field operators $\hat{\Psi}(\mathbf{x},t)$ and $\hat{\Psi}^\dagger(\mathbf{x},t)$ have together with (7.57), (7.58), and (7.72), the following consequences:

$$\begin{aligned}
\boldsymbol{\nabla}\hat{\Psi}(\mathbf{x},t) &= \frac{i}{\hbar}\sum_{r=1}^{2}\int d^3p\,\varepsilon_r\mathbf{p}\,\hat{a}_{\mathbf{p}}^{(r)}\,u_{\mathbf{p}}^{(r)}(\mathbf{x},t)\,, && (7.91)\\
\boldsymbol{\nabla}\hat{\Psi}^\dagger(\mathbf{x},t) &= -\frac{i}{\hbar}\sum_{r=1}^{2}\int d^3p\,\varepsilon_r\mathbf{p}\,\hat{a}_{\mathbf{p}}^{(r)\dagger}\,u_{\mathbf{p}}^{(r)*}(\mathbf{x},t)\,, && (7.92)\\
\hat{\Pi}(\mathbf{x},t) &= \frac{i\hbar}{2Mc^2}\sum_{r=1}^{2}\int d^3p\,\varepsilon_r E_{\mathbf{p}}\,\hat{a}_{\mathbf{p}}^{(r)\dagger}\,u_{\mathbf{p}}^{(r)*}(\mathbf{x},t)\,, && (7.93)\\
\hat{\Pi}^\dagger(\mathbf{x},t) &= \frac{-i\hbar}{2Mc^2}\sum_{r=1}^{2}\int d^3p\,\varepsilon_r E_{\mathbf{p}}\,\hat{a}_{\mathbf{p}}^{(r)}\,u_{\mathbf{p}}^{(r)}(\mathbf{x},t)\,. && (7.94)
\end{aligned}$$

Using now all plane wave expansions (7.71), (7.81) and (7.91)–(7.94) in the Hamilton operator of the Klein-Gordon field (7.56) we get at first

$$\begin{aligned}
\hat{H} &= \sum_{r=1}^{2}\sum_{r'=1}^{2}\int d^3p\int d^3p'\left(\frac{\varepsilon_r\varepsilon_{r'}E_{\mathbf{p}}E'_{\mathbf{p}}}{2Mc^2}+\frac{\varepsilon_r\varepsilon_{r'}\mathbf{p}\mathbf{p}'}{2M}+\frac{Mc^2}{2}\right)\hat{a}_{\mathbf{p}}^{(r)\dagger}\hat{a}_{\mathbf{p}'}^{(r')}\\
&\quad\times\int d^3x\,u_{\mathbf{p}}^{(r)*}(\mathbf{x},t)\,u_{\mathbf{p}'}^{(r')}(\mathbf{x},t)\,. && (7.95)
\end{aligned}$$

The remaining spatial integral is evaluated with (7.67), (7.72), and (7.78), yielding

$$\int d^3x\,u_{\mathbf{p}}^{(r)*}(\mathbf{x},t)\,u_{\mathbf{p}'}^{(r')}(\mathbf{x},t)=\frac{Mc^2}{E_{\mathbf{p}}}\,\exp\left\{\frac{i}{\hbar}\left(\varepsilon_r-\varepsilon_{r'}\right)E_{\mathbf{p}}t\right\}\,\delta(\mathbf{p}'-\varepsilon_r\varepsilon_{r'}\mathbf{p})\,. \tag{7.96}$$

Inserting (7.96) into (7.95) the integration with respect to the momenta $\mathbf{p}'$ can be evaluated by taking into account the symmetry (7.67)

$$\hat{H}=\sum_{r=1}^{2}\sum_{r'=1}^{2}\int d^3p\left(\frac{\varepsilon_r\varepsilon_{r'}E_{\mathbf{p}}^2}{2Mc^2}+\frac{\mathbf{p}^2}{2M}+\frac{Mc^2}{2}\right)\frac{Mc^2}{E_{\mathbf{p}}}\,\exp\left\{\frac{i}{\hbar}\left(\varepsilon_r-\varepsilon_{r'}\right)E_{\mathbf{p}}t\right\}\,\hat{a}_{\mathbf{p}}^{(r)\dagger}\hat{a}_{\varepsilon_r\varepsilon_{r'}\mathbf{p}}^{(r')}\,. \tag{7.97}$$

With the relativistic energy-momentum dispersion (7.66) this simplifies to

$$\hat{H}=\sum_{r=1}^{2}\sum_{r'=1}^{2}\int d^3p\,\frac{\varepsilon_r\varepsilon_{r'}+1}{2}\,E_{\mathbf{p}}\,\exp\left\{\frac{i}{\hbar}\left(\varepsilon_r-\varepsilon_{r'}\right)E_{\mathbf{p}}t\right\}\,\hat{a}_{\mathbf{p}}^{(r)\dagger}\hat{a}_{\varepsilon_r\varepsilon_{r'}\mathbf{p}}^{(r')}\,. \tag{7.98}$$

As Eq. (7.73) implies the auxiliary calculation

$$\frac{\varepsilon_r\varepsilon_{r'}+1}{2}=\begin{cases}1; & r=r'\\ 0; & r\neq r'\end{cases}=\delta_{r,r'}\;, \tag{7.99}$$

the Hamilton operator of the Klein-Gordon field (7.98) finally reduces to

$$\hat{H}=\sum_{r=1}^{2}\int d^3p\,E_{\mathbf{p}}\,\hat{a}_{\mathbf{p}}^{(r)\dagger}\hat{a}_{\mathbf{p}}^{(r)}\,. \tag{7.100}$$

Thus, whereas the intermediate results (7.97) and (7.98) suggest that the second-quantized Hamilton operator $\hat{H}$ of the Klein-Gordon theory may explicitly depend on time, the result (7.100) reveals that it turns out to be time-independent. This is consistent with the fact that the energy of the Klein-Gordon theory is a conserved quantity due its time translational invariance.

7.7 Charge Operator

According to (7.37), (7.39) and (7.42), (7.47), respectively, the charge of the Klein-Gordon field is defined by

$$Q = \frac{i\hbar}{2Mc^2} \int d^3x \left\{ \Psi^*(\mathbf{x},t) \frac{\partial \Psi(\mathbf{x},t)}{\partial t} - \frac{\partial \Psi^*(\mathbf{x},t)}{\partial t} \Psi(\mathbf{x},t) \right\} . \tag{7.101}$$

Due to (7.48) and (7.49) the charge (7.101) can be reexpressed as follows:

$$Q = \frac{i}{\hbar} \int d^3x \left\{ \Psi^*(\mathbf{x},t)\, \Pi^*(\mathbf{x},t) - \Pi(\mathbf{x},t)\, \Psi(\mathbf{x},t) \right\} . \tag{7.102}$$

Within the second quantization we assign to the charge a corresponding operator:

$$\hat{Q} = \frac{i}{\hbar} \int d^3x \left\{ \hat{\Psi}^\dagger(\mathbf{x},t)\, \hat{\Pi}^\dagger(\mathbf{x},t) - \hat{\Pi}(\mathbf{x},t)\, \hat{\Psi}(\mathbf{x},t) \right\} . \tag{7.103}$$

Note that here the respective order of the operators does play a role due to (7.53) and (7.54). The particular operator order chosen in (7.103) guarantees that the charge operator $\hat{Q}$ commutes with the Hamilton operator (7.56) due to applying (3.10) and (3.43):

$$\left[\hat{Q}, \hat{H} \right]_- = 0 . \tag{7.104}$$

Thus energy and charge remain to be both conserved quantities also in the second quantized Klein-Gordon theory. Inserting in (7.103) the plane wave expansions (7.71), (7.81) and (7.93), (7.94) we get at first

$$\hat{Q} \;=\; \sum_{r=1}^{2} \sum_{r'=1}^{2} \int d^3p \int d^3p' \, \frac{\varepsilon_r E_{\mathbf{p}} + \varepsilon_{r'} E_{\mathbf{p}'}}{2Mc^2} \, \hat{a}_{\mathbf{p}}^{(r)\dagger} \hat{a}_{\mathbf{p}'}^{(r')} \int d^3x \, u_{\mathbf{p}}^{(r)*}(\mathbf{x},t)\, u_{\mathbf{p}'}^{(r')}(\mathbf{x},t) . \tag{7.105}$$

Taking into account the symmetry (7.67), the integral (7.96), and the auxiliary calculation (7.77), the charge operator (7.105) reduces finally to the form

$$\hat{Q} = \sum_{r=1}^{2} \int d^3p \, \varepsilon_r \, \hat{a}_{\mathbf{p}}^{(r)\dagger} \hat{a}_{\mathbf{p}}^{(r)} . \tag{7.106}$$

Thus, also the charge operator $\hat{Q}$ turns out to be time independent, which confirms that the charge is a conserved quantity for the Klein-Gordon field.

7.8 Redefinition of Fourier Operators

Now we aim for a consistent physical interpretation of the results obtained so far within the second quantization of the Klein-Gordon field. From the commutation relations (7.88) and (7.90) we read off that the Fourier operators $\hat{a}_{\mathbf{p}}^{(1)}$, $\hat{a}_{\mathbf{p}}^{(2)\dagger}$ and $\hat{a}_{\mathbf{p}}^{(1)\dagger}$, $\hat{a}_{\mathbf{p}}^{(2)}$ have to be interpreted as annihilation operators and creation operators, respectively. This observation suggests to reinterpret the Fourier operators as follows:

$$\hat{a}_{\mathbf{p}} = \hat{a}_{\mathbf{p}}^{(1)} , \qquad \hat{a}_{\mathbf{p}}^{\dagger} = \hat{a}_{\mathbf{p}}^{(1)\dagger} , \qquad \hat{b}_{\mathbf{p}} = \hat{a}_{\mathbf{p}}^{(2)\dagger} , \qquad \hat{b}_{\mathbf{p}}^{\dagger} = \hat{a}_{\mathbf{p}}^{(2)} . \tag{7.107}$$

By using different letters a and b we express that the corresponding operators $\hat{a}_{\mathbf{p}}$, $\hat{b}_{\mathbf{p}}$ and $\hat{a}_{\mathbf{p}}^{\dagger}$, $\hat{b}_{\mathbf{p}}^{\dagger}$ describe the annihilation and the creation of different kinds of particles. Furthermore, this redefinition leaves the trivial commutation relations (7.88) invariant:

$$[\hat{a}_{\mathbf{p}}, \hat{a}_{\mathbf{p}'}]_- = \left[\hat{a}_{\mathbf{p}}^{\dagger}, \hat{a}_{\mathbf{p}'}^{\dagger}\right]_- = \left[\hat{b}_{\mathbf{p}}, \hat{b}_{\mathbf{p}'}\right]_- = \left[\hat{b}_{\mathbf{p}}^{\dagger}, \hat{b}_{\mathbf{p}'}^{\dagger}\right]_- = 0 , \tag{7.108}$$

$$\left[\hat{a}_{\mathbf{p}}, \hat{b}_{\mathbf{p}'}\right]_- = \left[\hat{a}_{\mathbf{p}}, \hat{b}_{\mathbf{p}'}^{\dagger}\right]_- = \left[\hat{a}_{\mathbf{p}}^{\dagger}, \hat{b}_{\mathbf{p}'}\right]_- = \left[\hat{a}_{\mathbf{p}}^{\dagger}, \hat{b}_{\mathbf{p}'}^{\dagger}\right]_- = 0 . \tag{7.109}$$

But the non-trivial commutation relations (7.90) are converted to

$$\left[\hat{a}_{\mathbf{p}}, \hat{a}_{\mathbf{p}'}^{\dagger}\right]_- = \left[\hat{b}_{\mathbf{p}}, \hat{b}_{\mathbf{p}'}^{\dagger}\right]_- = \delta(\mathbf{p} - \mathbf{p}') . \tag{7.110}$$

And the plane wave expansions (7.71) and (7.81) of the field operators $\hat{\Psi}(\mathbf{x}, t)$ and $\hat{\Psi}^{\dagger}(\mathbf{x}, t)$ then read due to (7.79):

$$\hat{\Psi}(\mathbf{x}, t) = \int d^3p \left\{ \hat{a}_{\mathbf{p}}\, u_{\mathbf{p}}(\mathbf{x}, t) + \hat{b}_{p}^{\dagger}\, u^*(\mathbf{x}, t) \right\} , \tag{7.111}$$

$$\hat{\Psi}^{\dagger}(\mathbf{x}, t) = \int d^3p \left\{ \hat{a}_{\mathbf{p}}^{\dagger}\, u_{\mathbf{p}}^*(\mathbf{x}, t) + \hat{b}_{p}\, u(\mathbf{x}, t) \right\} . \tag{7.112}$$

Here we have introduced according to (7.72) and (7.78)

$$u_{\mathbf{p}}(\mathbf{x}, t) = u_{\mathbf{p}}^{(1)}(\mathbf{x}, t) = \sqrt{\frac{Mc^2}{(2\pi\hbar)^3 E_{\mathbf{p}}}} \exp\left\{ \frac{i}{\hbar} \left(\mathbf{p}\mathbf{x} - E_{\mathbf{p}} t\right) \right\} . \tag{7.113}$$

In addition, the Hamilton operator (7.100) and the charge operator (7.106) read due to the redefinition (7.107)

$$\hat{H} = \int d^3p\, E_{\mathbf{p}} \left(\hat{a}_{\mathbf{p}}^{\dagger} \hat{a}_{\mathbf{p}} + \hat{b}_{\mathbf{p}} \hat{b}_{\mathbf{p}}^{\dagger} \right) , \tag{7.114}$$

$$\hat{Q} = \int d^3p \left(\hat{a}_{\mathbf{p}}^{\dagger} \hat{a}_{\mathbf{p}} - \hat{b}_{\mathbf{p}} \hat{b}_{\mathbf{p}}^{\dagger} \right) . \tag{7.115}$$

In order to obtain a normal ordering of the operators we have to use the commutator (7.110), yielding

$$\hat{H} = \int d^3p\, E_{\mathbf{p}} \left(\hat{a}_{\mathbf{p}}^{\dagger} \hat{a}_{\mathbf{p}} + \hat{b}_{\mathbf{p}}^{\dagger} \hat{b}_{\mathbf{p}} \right) + \delta(\mathbf{0}) \int d^3p\, E_{\mathbf{p}} , \tag{7.116}$$

$$\hat{Q} = \int d^3p \left(\hat{a}_{\mathbf{p}}^{\dagger} \hat{a}_{\mathbf{p}} - \hat{b}_{\mathbf{p}}^{\dagger} \hat{b}_{\mathbf{p}} \right) - \delta(\mathbf{0}) \int d^3p . \tag{7.117}$$

The vacuum state is defined here as usual

$$\hat{a}_{\mathbf{p}}|0\rangle = 0\,, \qquad \hat{b}_{\mathbf{p}}|0\rangle = 0\,. \tag{7.118}$$

With this the vacuum expectation values of both the Hamilton operator and the charge operator result to

$$\langle 0|\hat{H}|0\rangle = \delta(\mathbf{0}) \int d^3p\, E_{\mathbf{p}}\,, \tag{7.119}$$

$$\langle 0|\hat{Q}|0\rangle = -\delta(\mathbf{0}) \int d^3p\,, \tag{7.120}$$

which are divergent due to two reasons. On the one hand the factor $\delta(\mathbf{0})$ is divergent and on the other hand the respective momentum integrals are divergent as well. Therefore, one considers instead of the Hamilton operator and the charge operator the respective renormalized quantities:

$$:\hat{H}: \;=\; \hat{H} - \langle 0|\hat{H}|0\rangle = \int d^3p\, E_{\mathbf{p}} \left(\hat{a}^\dagger_{\mathbf{p}}\hat{a}_{\mathbf{p}} + \hat{b}^\dagger_{\mathbf{p}}\hat{b}_{\mathbf{p}}\right), \tag{7.121}$$

$$:\hat{Q}: \;=\; \hat{Q} - \langle 0|\hat{Q}|0\rangle = \int d^3p \left(\hat{a}^\dagger_{\mathbf{p}}\hat{a}_{\mathbf{p}} - \hat{b}^\dagger_{\mathbf{p}}\hat{b}_{\mathbf{p}}\right). \tag{7.122}$$

We recognize that both renormalized operators $:\langle 0|\hat{H}|0\rangle:$ and $:\langle 0|\hat{Q}|0\rangle:$ are normal ordered, i.e. the creation (annihilation) operators stand on the left-hand (right-hand) side.

The results (7.121) and (7.122) allow now for the following physical interpretation. The operators $\hat{a}^\dagger_{\mathbf{p}}$, $\hat{a}_{\mathbf{p}}$ ($\hat{b}^\dagger_{\mathbf{p}}$, $\hat{b}_{\mathbf{p}}$) describe particles of charge 1 (-1) and energy $E_{\mathbf{p}}$. As the two particle types only differ by their charge, they represent particles and their respective antiparticles. The particle type a (b) can be identified with the pion π^+ (π^-). On the basis of this insight, we recognize in (7.111) that the field operator $\hat{\Psi}(\mathbf{x},t)$ contains both the annihilation of particles a with charge 1 and the creation of antiparticles b with charge -1. These microscopic processes act together such that the field operator $\hat{\Psi}(\mathbf{x},t)$ describes the annihilation of a charge 1 and, correspondingly, the adjoint field operator $\hat{\Psi}^\dagger(\mathbf{x},t)$ represents the creation of a charge 1 at the space-point $(\mathbf{x},t)$. This physical interpretation of the second-quantized operators $\hat{\Psi}(\mathbf{x},t)$ and $\hat{\Psi}^\dagger(\mathbf{x},t)$ turns out to be crucial for the corresponding propagator of the Klein-Gordon theory.

7.9 Definition of Propagator

In the following we investigate in more detail the Klein-Gordon propagator, which is an important ingredient of quantum field theory when the interaction of the Klein-Gordon field with other quantum fields is treated perturbatively. For instance, the Klein-Gordon propagator is an essential building block of scalar quantum electrodynamics, where the photon exchange between charged pions is described graphically in terms of corresponding Feynman diagrams. But the Klein-Gordon propagator turns out to be also central for this lecture from a technical point of view. On the one hand, its non-relativistic limit leads to the Schrödinger propagator, which is discussed in detail in Appendix A and is used in the context of non-relativistic quantum many-body theory. On the other hand, we will see later on that the propagator of the Dirac theory is determined by partial derivatives from the Klein-Gordon propagator. Thus, having a profound understanding of the Klein-Gordon propagator represents a prerequisite for the Dirac propagator, which is a key element of the Feynman diagrams of quantum electrodynamics.

Let us start with defining the Klein-Gordon propagator as the vacuum expectation value of the product of two field operators:

$$G(\mathbf{x},t;\mathbf{x}',t') = \left\langle 0 \left| \hat{T}\left(\hat{\Psi}(\mathbf{x},t)\,\hat{\Psi}^\dagger(\mathbf{x}',t')\right)\right| 0\right\rangle . \tag{7.123}$$

The symbol $\hat{T}$ denotes the time-ordered product of the field operators $\hat{\Psi}(\mathbf{x},t)$ and $\hat{\Psi}^\dagger(\mathbf{x}',t')$. Given two time-dependent bosonic operators $\hat{A}(t)$ and $\hat{B}(t')$, their time-ordered product reads

$$\hat{T}\left(\hat{A}(t)\,\hat{B}(t')\right) = \Theta(t-t')\,\hat{A}(t)\,\hat{B}(t') + \Theta(t'-t)\,\hat{B}(t')\,\hat{A}(t)\,, \tag{7.124}$$

where we have used the Heaviside function

$$\Theta(t) = \begin{cases} 1\,; & t>0 \\ 0\,; & t<0 \end{cases} . \tag{7.125}$$

Thus, the operator-valued factors in (7.124) are put into chronological order so that the operator having the later time argument is put first, i.e. to the left. If the two time arguments happen to be equal, problems might arise since the operator ordering is then not well defined. In the present case (7.123), however, this is not the case since the operators $\hat{\Psi}(\mathbf{x},t)$ and $\hat{\Psi}^\dagger(\mathbf{x}',t)$ at equal time commute due to (7.55). Taking into account (7.124) in (7.123) leads to

$$G(\mathbf{x},t;\mathbf{x}',t') = \Theta(t-t')\left\langle 0\left|\hat{\Psi}(\mathbf{x},t)\,\hat{\Psi}^\dagger(\mathbf{x}',t')\right|0\right\rangle + \Theta(t'-t)\left\langle 0\left|\hat{\Psi}^\dagger(\mathbf{x}',t')\,\hat{\Psi}(\mathbf{x},t)\right|0\right\rangle . \tag{7.126}$$

Note that this introduction of the Klein-Gordon propagator with a time-ordered product of field operators appears admittedly to be quite unmotivated at this stage of the lecture. But it will be justified a posteriori when dealing perturbatively with interacting quantum fields. Namely, such a perturbative treatment is performed systematically in the so-called Dirac interaction picture, where the unperturbed Hamiltonian determines the time dependence of the field operators, so that their interpretation of representing creation and annihilation operators is preserved, and the perturbative Hamiltonian affects the quantum states. And the latter turns out to lead to the time evolution operator in the Dirac interaction picture, whose perturbative expansion naturally involves the time-ordered product of field operators. Thus, in conclusion, any perturbative treatment in quantum field theory is based on the time-ordered product of field operators.

In order to determine the equation of motion for the Klein-Gordon propagator we calculate the first time derivative:

$$\frac{\partial G(\mathbf{x},t;\mathbf{x}',t')}{\partial t} = \delta(t-t')\left\langle 0\left|\left[\hat{\Psi}(\mathbf{x},t),\hat{\Psi}^\dagger(\mathbf{x}',t')\right]_-\right|0\right\rangle \tag{7.127}$$
$$+\Theta(t-t')\left\langle 0\left|\frac{\partial\hat{\Psi}(\mathbf{x},t)}{\partial t}\,\hat{\Psi}^\dagger(\mathbf{x}',t')\right|0\right\rangle + \Theta(t'-t)\left\langle 0\left|\hat{\Psi}^\dagger(\mathbf{x}',t')\,\frac{\partial\hat{\Psi}(\mathbf{x},t)}{\partial t}\right|0\right\rangle .$$

Here we have used that the fact that the time derivative of the Heaviside function yields the delta function:

$$\frac{\partial \Theta(t)}{\partial t} = \delta(t)\,. \tag{7.128}$$

As the commutator of the field operators $\hat{\Psi}(\mathbf{x}, t)$ and $\hat{\Psi}^\dagger(\mathbf{x}', t)$ at the same time t vanish according to (7.55), the first term in (7.127) goes away. Another time derivative leads then with (7.128) to

$$\frac{\partial^2 G(\mathbf{x}, t; \mathbf{x}', t')}{\partial t^2} = \delta(t - t') \left\langle 0 \right| \left[\frac{\partial \hat{\Psi}(\mathbf{x}, t)}{\partial t}, \hat{\Psi}^\dagger(\mathbf{x}', t') \right]_- \left| 0 \right\rangle \tag{7.129}$$

$$+\Theta(t - t') \left\langle 0 \left| \frac{\partial^2 \hat{\Psi}(\mathbf{x}, t)}{\partial t^2} \, \hat{\Psi}^\dagger(\mathbf{x}', t') \right| 0 \right\rangle + \Theta(t' - t) \left\langle 0 \left| \hat{\Psi}^\dagger(\mathbf{x}', t') \, \frac{\partial^2 \hat{\Psi}(\mathbf{x}, t)}{\partial t^2} \right| 0 \right\rangle \,.$$

Taking into account (7.54), (7.57), (7.61), and (7.126) we finally obtain

$$\left(\frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \Delta + \frac{M^2 c^2}{\hbar^2} \right) G(\mathbf{x}, t; \mathbf{x}', t') = -i \, \frac{2M}{\hbar} \, \delta(t - t') \, \delta(\mathbf{x} - \mathbf{x}')\,. \tag{7.130}$$

Thus, we recognize that the Klein-Gordon propagator represents the Green function of the Klein-Gordon equation. As a coupling of the Klein-Gordon field to other quantum fields yields as a Heisenberg equation an inhomogeneous Klein-Gordon equation, its perturbative solution is based on the knowledge of the corresponding Green function, i.e. the Klein-Gordon propagator.

In view of the non-relativistic limit $c \to \infty$ we have to separate the rest energy from the Klein-Gordon propagator due to (7.5):

$$G(\mathbf{x}, t; \mathbf{x}', t') = g(\mathbf{x}, t; \mathbf{x}', t') \, \exp\left(-\frac{i}{\hbar} \, M c^2 t \right) \,. \tag{7.131}$$

Inserting the ansatz (7.131) in the equation of motion (7.130) we get

$$\left(\frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \frac{2iM}{\hbar} \frac{\partial}{\partial t} - \Delta \right) g(\mathbf{x}, t; \mathbf{x}', t') = -i \, \frac{2M}{\hbar} \, \delta(t - t') \, \delta(\mathbf{x} - \mathbf{x}')\,. \tag{7.132}$$

Performing then the non-relativistic limit $c \to \infty$ Eq. (7.132) reduces to

$$\left(i\hbar \, \frac{\partial}{\partial t} + \frac{\hbar^2}{2M} \, \Delta \right) g(\mathbf{x}, t; \mathbf{x}', t') = i\hbar \, \delta(t - t') \, \delta(\mathbf{x} - \mathbf{x}')\,. \tag{7.133}$$

Thus, $g(\mathbf{x}, t; \mathbf{x}', t')$ coincides with the Green function of the Schrödinger equation and can be identified with the Schrödinger propagator discussed in the exercises.

7.10 Interpretation of Propagator

Now we deal with the physical interpretation of the Klein-Gordon propagator (7.126). To this end we state two commutation relations for the charge operator (7.103):

$$\left[\hat{Q}, \hat{\Psi}(\mathbf{x}, t) \right]_- = -\hat{\Psi}(\mathbf{x}, t)\,, \tag{7.134}$$

$$\left[\hat{Q}, \hat{\Psi}^\dagger(\mathbf{x}, t) \right]_- = \hat{\Psi}^\dagger(\mathbf{x}, t)\,. \tag{7.135}$$

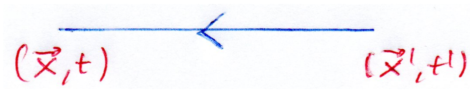

Figure 7.3: Graphical representation of the Klein-Gordon propagator (7.126) describing the propagation of the charge 1 from $(\mathbf{x}', t')$ to $(\mathbf{x}, t)$.

Thus, the field operators $\hat{\Psi}(\mathbf{x}, t)$ and $\hat{\Psi}^\dagger(\mathbf{x}, t)$ decrease and increase the charge by one unit, respectively, as was already anticipated at the end of Section 7.8. Namely, denoting with $|q\rangle$ an eigenstate of the charge operator $\hat{Q}$ with eigenvalue q, i.e.

$$\hat{Q}|q\rangle = q\,|q\rangle\,, \tag{7.136}$$

we conclude with the help of the commutator relations (7.134), (7.135):

$$\hat{Q}\hat{\Psi}(\mathbf{x}, t)|q\rangle = \hat{\Psi}(\mathbf{x}, t)\big(\hat{Q} - 1\big)|q\rangle = (q-1)\hat{\Psi}(\mathbf{x}, t)|q\rangle \quad \Longrightarrow \quad |q-1\rangle \sim \hat{\Psi}(\mathbf{x}, t)|q\rangle\,, \tag{7.137}$$

$$\hat{Q}\hat{\Psi}^\dagger(\mathbf{x}, t)|q\rangle = \hat{\Psi}^\dagger(\mathbf{x}, t)\big(\hat{Q} + 1\big)|q\rangle = (q+1)\hat{\Psi}^\dagger(\mathbf{x}, t)|q\rangle \quad \Longrightarrow \quad |q+1\rangle \sim \hat{\Psi}^\dagger(\mathbf{x}, t)|q\rangle\,. \tag{7.138}$$

Against this background the Klein-Gordon propagator (7.126) describes the propagation of the charge 1 from $(\mathbf{x}', t')$ to $(\mathbf{x}, t)$, see Fig. 7.3, via two microscopic processes. Taking into account the plane wave decompositions (7.111), (7.112) the first term in (7.126) describes the propagation of a particle of charge $+1$ from $(\mathbf{x}', t')$ to $(\mathbf{x}, t)$, whereas the second term considers the propagation of an antiparticle of charge -1 from $(\mathbf{x}, t)$ to $(\mathbf{x}', t')$. Thus, the Klein-Gordon propagator (7.126) takes both processes of particle and antiparticle propagation into account. But, according to the intuitive physical picture of Richard Feynman, particles with positive energy propagate forward in time, whereas antiparticles are considered to have negative energy, which move backwards in time.

7.11 Calculation of Propagator

Now we insert the plane wave decompositions (7.111), (7.112) of the field operators $\hat{\Psi}(\mathbf{x}, t)$, $\hat{\Psi}^\dagger(\mathbf{x}, t)$ into the definition of the Klein-Gordon propagator (7.126). Due to the commutation relations (7.108)–(7.110) and the definition of the vacuum state (7.118) we obtain the plane wave representation

$$G(\mathbf{x}, t; \mathbf{x}', t') = \int d^3p \left\{\Theta(t-t')u_{\mathbf{p}}(\mathbf{x}, t)u_{\mathbf{p}}^*(\mathbf{x}', t') + \Theta(t'-t)u_{\mathbf{p}}(\mathbf{x}', t')u_{\mathbf{p}}^*(\mathbf{x}, t)\right\}. \tag{7.139}$$

Inserting the plane wave (7.113) together with the relativistic energy-momentum dispersion (7.66), one obtains the following Fourier representation of the Klein-Gordon propagator:

$$\begin{aligned} G(\mathbf{x},t;\mathbf{x}',t') &= \frac{Mc^2}{(2\pi\hbar)^3}\int d^3p\,\frac{1}{\sqrt{\mathbf{p}^2c^2+M^2c^4}} \\ &\quad\times\left(\Theta(t-t')\,\exp\left\{\frac{i}{\hbar}\left[\mathbf{p}(\mathbf{x}-\mathbf{x}')-\sqrt{\mathbf{p}^2c^2+M^2c^4}\,(t-t')\right]\right\}\right. \\ &\quad\left.+\Theta(t'-t)\,\exp\left\{\frac{i}{\hbar}\left[\mathbf{p}(\mathbf{x}'-\mathbf{x})-\sqrt{\mathbf{p}^2c^2+M^2c^4}\,(t'-t)\right]\right\}\right). \end{aligned} \tag{7.140}$$

In the following we evaluate this momentum integral analytically. At first, substituting in the second term $\mathbf{p}\to-\mathbf{p}$, both terms are combined as follows:

$$\begin{aligned} G(\mathbf{x},t;\mathbf{x}',t') &= \frac{Mc^2}{(2\pi\hbar)^3}\int d^3p\,\frac{1}{\sqrt{\mathbf{p}^2c^2+M^2c^4}} \\ &\quad\times\exp\left\{\frac{i}{\hbar}\,\mathbf{p}(\mathbf{x}-\mathbf{x}')-\frac{i}{\hbar}\sqrt{\mathbf{p}^2c^2+M^2c^4}\,|t-t'|\right\}. \end{aligned} \tag{7.141}$$

Introducing subsequently spherical coordinates for the momentum integral, we obtain at first

$$\begin{aligned} G(\mathbf{x},t;\mathbf{x}',t') &= \frac{Mc^2}{(2\pi\hbar)^3}\int_0^{2\pi}d\varphi\int_0^{\pi}d\theta\sin\theta\int_0^{\infty}dp\,p^2\,\frac{1}{\sqrt{p^2c^2+M^2c^4}} \\ &\quad\times\exp\left\{\frac{i}{\hbar}\,p|\mathbf{x}-\mathbf{x}'|\,\cos\theta-\frac{i}{\hbar}\,\sqrt{p^2c^2+M^2c^4}\,|t-t'|\right\}. \end{aligned} \tag{7.142}$$

Evaluating the angle integrals explicitly, one gets two remaining integrals over the absolute value of the momentum. Performing the substitution $p\to-p$ in the second integral, both integrals over half axis can be combined into a single one over the whole real axis, yielding

$$\begin{aligned} G(\mathbf{x},t;\mathbf{x}',t') &= \frac{-iMc^2}{4\pi^2\hbar^2|\mathbf{x}-\mathbf{x}'|}\int_{-\infty}^{\infty}dp\,\frac{p}{\sqrt{p^2c^2+M^2c^4}} \\ &\quad\times\exp\left\{\frac{i}{\hbar}\left[p|\mathbf{x}-\mathbf{x}'|-\sqrt{p^2c^2+M^2c^4}\,|t-t'|\right]\right\}. \end{aligned} \tag{7.143}$$

Here the factor p in the integrand can be represented in terms of a partial derivative with respect to the distance $|\mathbf{x}-\mathbf{x}'|$:

$$\begin{aligned} G(\mathbf{x},t;\mathbf{x}',t') &= \frac{-Mc^2}{4\pi^2\hbar|\mathbf{x}-\mathbf{x}'|}\,\frac{\partial}{\partial|\mathbf{x}-\mathbf{x}'|}\int_{-\infty}^{\infty}dp\,\frac{1}{\sqrt{p^2c^2+M^2c^4}} \\ &\quad\times\exp\left\{\frac{i}{\hbar}\left[p|\mathbf{x}-\mathbf{x}'|-\sqrt{p^2c^2+M^2c^4}\,|t-t'|\right]\right\}. \end{aligned} \tag{7.144}$$

Due to the substitution

$$p\,(z)=Mc\sinh z\,, \tag{7.145}$$

where we have

$$\frac{dp\,(z)}{dz}=Mc\cosh z=Mc\sqrt{1+\sinh^2 z}=\frac{1}{c}\,\sqrt{p^2c^2+M^2c^4}\,, \tag{7.146}$$

Eq. (7.144) is converted to

$$\begin{aligned} G(\mathbf{x},t;\mathbf{x}',t') &= \frac{-Mc}{4\pi^2\hbar|\mathbf{x}-\mathbf{x}'|}\,\frac{\partial}{\partial|\mathbf{x}-\mathbf{x}'|} \\ &\quad\times\int_{-\infty}^{\infty} dz\,\exp\left\{\frac{iMc}{\hbar}\left[|\mathbf{x}-\mathbf{x}'|\sinh z - c|t-t'|\cosh z\right]\right\}\,. \end{aligned} \tag{7.147}$$

We now aim at simplifying the integral (7.147) by combining the two terms in the argument of the exponential function into a single one. This is accomplished by the trick to perform the substitution $z = z' + z_0$, which introduces a new variable z_0 into the calculation:

$$\begin{aligned} G(\mathbf{x},t;\mathbf{x}',t') = \frac{-Mc}{4\pi^2\hbar|\mathbf{x}-\mathbf{x}'|}\,\frac{\partial}{\partial|\mathbf{x}-\mathbf{x}'|} \\ \times\int_{-\infty}^{\infty} dz\,\exp\left\{\frac{iMc}{\hbar}\left[|\mathbf{x}-\mathbf{x}'|\sinh(z+z_0) - c|t-t'|\cosh(z+z_0)\right]\right\}\,. \end{aligned} \tag{7.148}$$

Taking into account the addition theorems of hyperbolic functions

$$\sinh(z+z_0) = \sinh z\,\cosh z_0 + \cosh z\,\sinh z_0\,, \tag{7.149}$$

$$\cosh(z+z_0) = \cosh z\,\cosh z_0 + \sinh z\,\sinh z_0\,, \tag{7.150}$$

the integral (7.148) gets at first more involved:

$$\begin{aligned} G(\mathbf{x},t;\mathbf{x}',t') &= \frac{-Mc}{4\pi^2\hbar|\mathbf{x}-\mathbf{x}'|}\,\frac{\partial}{\partial|\mathbf{x}-\mathbf{x}'|}\int_{-\infty}^{\infty} dz \\ &\quad\times\exp\left\{\frac{iMc}{\hbar}\left[\Big(|\mathbf{x}-\mathbf{x}'|\cosh z_0 - c|t-t'|\sinh z_0\Big)\sinh z\right.\right. \\ &\quad\left.\left.+\Big(|\mathbf{x}-\mathbf{x}'|\sinh z_0 - c|t-t'|\cosh z_0\Big)\cosh z\right]\right\}\,. \end{aligned} \tag{7.151}$$

But a closer inspection then reveals that the yet undetermined parameter z_0 can be chosen in such a way that the argument of the exponential function in (7.151) does only depend on one term, for instance on the $\cosh z$ function:

$$\tanh z_0 = \frac{\sinh z_0}{\cosh z_0} = \frac{|\mathbf{x}-\mathbf{x}'|}{c|t-t'|}\,. \tag{7.152}$$

The subsequent hyperbolic side calculations

$$\sinh z_0 = \frac{\tanh z_0}{\sqrt{1-\tanh^2 z_0}} = \frac{|\mathbf{x}-\mathbf{x}'|}{\sqrt{c^2(t-t')^2-(\mathbf{x}-\mathbf{x}')^2}}\,, \tag{7.153}$$

$$\cosh z_0 = \frac{1}{\sqrt{1-\tanh^2 z_0}} = \frac{c|t-t'|}{\sqrt{c^2(t-t')^2-(\mathbf{x}-\mathbf{x}')^2}} \tag{7.154}$$

together with (7.152) then simplify the integral in (7.151) to

$$\begin{aligned} G(\mathbf{x},t;\mathbf{x}',t') &= \frac{-Mc}{4\pi^2\hbar|\mathbf{x}-\mathbf{x}'|}\,\frac{\partial}{\partial|\mathbf{x}-\mathbf{x}'|}\int_{-\infty}^{\infty} dz \\ &\quad\times\exp\left\{-i\,\frac{Mc}{\hbar}\sqrt{c^2(t-t')^2-(\mathbf{x}-\mathbf{x}')^2}\,\cosh z\right\}\,. \end{aligned} \tag{7.155}$$

Here we can use the Hankel function of second kind [(8.405.2), Gradshteyn/Ryzhik]

$$H_\nu^{(2)}(x) = J_\nu(x) - iN_\nu(x)\,, \tag{7.156}$$

which consists of the Bessel function $J_\nu(x)$ and the von Neumann function $N_\nu(x)$, due to its integral representation [(8.421.2), Gradshteyn/Ryzhik]

$$H_\nu^{(2)}(x) = -\frac{e^{i\nu\pi/2}}{\pi\, i}\int_{-\infty}^{\infty} dt\, e^{-ix\cosh t - \nu t}\,. \tag{7.157}$$

With this we obtain from (7.155)

$$G(\mathbf{x},t;\mathbf{x}',t') = \frac{iMc}{4\pi\hbar|\mathbf{x}-\mathbf{x}'|}\,\frac{\partial}{\partial|\mathbf{x}-\mathbf{x}'|}\,H_0^{(2)}\left(\frac{Mc}{\hbar}\sqrt{c^2\,(t-t')^2-(\mathbf{x}-\mathbf{x}')^2}\right)\,. \tag{7.158}$$

Thus, it remains to evaluate the derivative, where we have to take into account [(8.473.6), Gradshteyn/Ryzhik]

$$\frac{d}{dx}\,H_0^{(2)}(x) = -H_1^{(2)}(x)\,. \tag{7.159}$$

Thus we get for the Klein-Gordon propagator the following explicit result:

$$G(\mathbf{x},t;\mathbf{x}',t') = \frac{i(Mc/\hbar)^2}{4\pi\sqrt{c^2\,(t-t')^2-(\mathbf{x}-\mathbf{x}')^2}}\,H_1^{(2)}\left(\frac{Mc}{\hbar}\sqrt{c^2\,(t-t')^2-(\mathbf{x}-\mathbf{x}')^2}\right)\,. \tag{7.160}$$

We note that the particle M enters here only in form of the Compton wave length (7.21).

In the non-relativistic limit $c\to\infty$ the argument of the Hankel function becomes arbitrarily large, so we we use [(8.451.4), Gradshtey/Ryzhik]:

$$H_\nu^{(2)}(x) \approx \sqrt{\frac{2}{\pi x}}\,e^{-i\left(x-\frac{\pi}{2}\nu-\frac{\pi}{4}\right)}\,, \qquad x \gg 1\,. \tag{7.161}$$

With this the non-relativistic limit of the Klein-Gordon propagator (7.160) is for $t > t'$ of the form (7.131) with

$$g(\mathbf{x},t;\mathbf{x}',t') = \sqrt{\left(\frac{M}{2\pi i\hbar\,(t-t')}\right)^3}\,\exp\left\{\frac{iM\,(\mathbf{x}-\mathbf{x}')^2}{2\hbar\,(t-t')}\right\}. \tag{7.162}$$

According to the exercises Eq. (7.162) represents the solution of the inhomogeneous Schrödinger equation (7.133). Thus, indeed, the Klein-Gordon propagator reduces in the non-relativistic limit to the Schrödinger propagator.

7.12 Covariant Form of Propagator

In view of obtaining a manifestly covariant form of the Klein-Gordon propagator, we extend now its three-dimensional Fourier representation (7.141) to a four-dimensional one. To this end we consider the integral

$$I\,(t-t') \;=\; \lim_{\eta\downarrow 0}\int_{-\infty}^{\infty}\frac{dE}{2\pi\hbar}\,\frac{e^{-\frac{i}{\hbar}E(t-t')}}{E^2-E_{\mathbf{p}}^2+i\eta}\,. \tag{7.163}$$

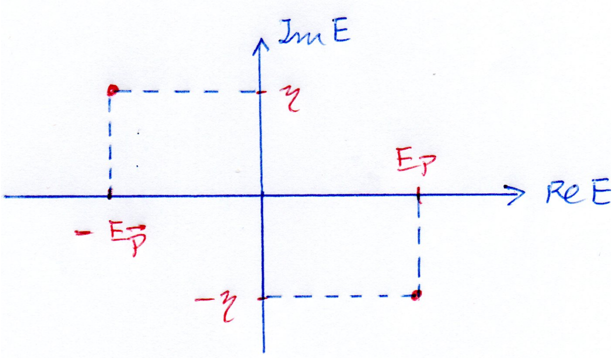

Figure 7.4: Shift of energy poles according to the $i\eta$ prescription of Richard Feynman.

Here the term $i\eta$ with $\eta > 0$ shifts infinitesimally the poles of the integrand on the real axis into the complex plane in a particular way. According to this $i\eta$ prescription, which was introduced by Richard Feynman, the pole at $E = E_{\mathbf{p}}$ is shifted below the real axis, whereas the pole at $E = -E_{\mathbf{p}}$ is shifted above the real axis, see Fig. 7.4. As we see in due course this guarantees that particles (antiparticles) move forward (backward) in time. To this end we evaluate the integral (7.163) with the help of the residue theorem. In order to guarantee the convergence of the integral one has to close the integration contour along the real axis for $t > t'$ ($t < t'$) in the lower (upper) part of the complex plane, yielding

$$t > t' : I\,(t-t') = \frac{-2\pi i}{2\pi\hbar} \lim_{\eta\downarrow 0} \operatorname*{Res}_{E=\sqrt{E_{\mathbf{p}}^2 - i\eta}} \frac{e^{-\frac{i}{\hbar}E(t-t')}}{E^2 - E_{\mathbf{p}}^2 + i\eta} = -\frac{i}{2\hbar E_{\mathbf{p}}}\, e^{-\frac{i}{\hbar}E_{\mathbf{p}}(t-t')}\,, \tag{7.164}$$

$$t < t' : I\,(t-t') = \frac{2\pi i}{2\pi\hbar} \lim_{\eta\downarrow 0} \operatorname*{Res}_{E=-\sqrt{E_{\mathbf{p}}^2 - i\eta}} \frac{e^{-\frac{i}{\hbar}E(t-t')}}{E^2 - E_{\mathbf{p}}^2 + i\eta} = -\frac{i}{2\hbar E_{\mathbf{p}}}\, e^{\frac{i}{\hbar}E_{\mathbf{p}}(t-t')}\,. \tag{7.165}$$

Here we have used the fact that the residue of a function $f(z)$ with a simple pole at $z = z_0$ is determined via

$$\operatorname*{Res}_{z\,=\,z_0} f(z) = \lim_{z\to z_0} (z - z_0)\, f(z)\,. \tag{7.166}$$

Both results (7.164), (7.165) can be summarized as follows:

$$I\,(t-t') = -\frac{i}{2\hbar E_{\mathbf{p}}} \left\{\Theta(t-t')\, e^{-\frac{i}{\hbar}E_{\mathbf{p}}(t-t')} + \Theta(t'-t)\, e^{\frac{i}{\hbar}E_{\mathbf{p}}(t-t')}\right\} = -\frac{i}{2\hbar E_{\mathbf{p}}}\, e^{-\frac{i}{\hbar}E_{\mathbf{p}}|t-t'|}\,. \tag{7.167}$$

Inserting (7.163) and (7.167) into (7.141) leads at first to

$$\begin{aligned} G(\mathbf{x}, t; \mathbf{x}', t') &= 2i\hbar M c^2 \lim_{\eta\downarrow 0} \int \frac{d^3p}{(2\pi\hbar)^3} \int \frac{dE}{2\pi\hbar}\, \frac{1}{E^2 - \mathbf{p}^2c^2 - M^2c^4 + i\eta} \\ &\quad \times \exp\left\{-\frac{i}{\hbar}\Big[E\,(t-t') - \mathbf{p}\,(\mathbf{x}-\mathbf{x}')\Big]\right\}. \end{aligned} \tag{7.168}$$

This can be rewritten in a manifestly Lorentz covariant form as follows:

$$G(x^\lambda; x'^\lambda) = 2i\hbar M c \lim_{\eta\downarrow 0} \int \frac{d^4p}{(2\pi\hbar)^4}\, \frac{1}{g_{\mu\nu}p^\mu p^\nu - M^2c^2 + i\eta}\, \exp\left\{-\frac{i}{\hbar}\, g_{\mu\nu}\, p^\mu\, (x^\nu - x'^\nu)\right\}. \tag{7.169}$$

In this form the equation of motion of the Klein-Gordon propagator (7.130) is obviously fulfilled:

$$\left(g_{\mu\nu}\hat{p}^\mu\hat{p}^\nu + \frac{M^2c^2}{\hbar^2} \right) G(x^\lambda; x'^\lambda) = 2i\hbar Mc \lim_{\eta\downarrow 0} \int \frac{d^4p}{(2\pi\hbar)^4} \frac{g_{\mu\nu}\,\frac{-i}{\hbar}\,p^\mu\,\frac{-i}{\hbar}\,p^\nu + \frac{M^2c^2}{\hbar^2}}{g_{\mu\nu}p^\mu p^\nu - M^2c^2 + i\eta}$$
$$\times \exp\left\{ -\frac{i}{\hbar}\, g_{\mu\nu}\, p^\mu \left(x^\nu - x'^\nu \right) \right\} = -\frac{2iMc}{\hbar} \int \frac{d^4p}{(2\pi\hbar)^4} \exp\left\{ -\frac{i}{\hbar}\, g_{\mu\nu}\, p^\mu \left(x^\nu - x'^\nu \right) \right\}$$
$$= -\frac{2iMc}{\hbar}\, \delta^{(4)}(x - x') = -\frac{2iM}{\hbar}\, \delta(t - t')\, \delta\left(\mathbf{x} - \mathbf{x}' \right) . \tag{7.170}$$

Comparing (7.169) with the four-dimensional Fourier transformation the Klein-Gordon propagator

$$G(x^\lambda; x'^\lambda) = \int \frac{d^4p}{(2\pi\hbar)^4}\, G(p^\lambda)\, \exp\left\{ -\frac{i}{\hbar}\, g_{\mu\nu}\, p^\mu \left(x^\nu - x'^\nu \right) \right\} , \tag{7.171}$$

we read off

$$G(p^\lambda) = G(\mathbf{p}, E) = \lim_{\eta\downarrow 0} \frac{2i\hbar Mc}{E^2 - \mathbf{p}^2c^2 - M^2c^4 + i\eta} . \tag{7.172}$$

Here a singularity appears when the energy variable E coincides with the physical energy of a relativistic massive particle, which is given by the energy-momentum dispersion (7.66). In the non-relativistic limit $c \to \infty$ the Fourier transformed of the Klein-Gordon propagator (7.172) goes over into the Fourier transformed of the Schrödinger propagator:

$$\begin{aligned} g(\mathbf{p}, E) &= \lim_{c\to\infty} \frac{1}{c}\, G(\mathbf{p}, E + Mc^2) = \lim_{\eta\downarrow 0}\, \lim_{c\to\infty} \frac{2i\hbar M}{(E/c + Mc)^2 - \mathbf{p}^2 - M^2c^2 + i\eta} \\ &= \lim_{\eta\downarrow 0}\, \lim_{c\to\infty} \frac{i\hbar}{E - \frac{\mathbf{p}^2}{2M} + \frac{E^2}{2Mc^2} + i\eta} = \lim_{\eta\downarrow 0} \frac{i\hbar}{E - \frac{\mathbf{p}^2}{2M} + i\eta} . \end{aligned} \tag{7.173}$$

Indeed, solving the inhomogeneous Schrödinger equation (7.133) via a four-dimensional Fourier transformation

$$g(\mathbf{x}, t; \mathbf{x}', t') = \int_{-\infty}^{\infty} \frac{dE}{2\pi\hbar} \int \frac{d^3p}{(2\pi\hbar)^3}\, g(\mathbf{p}, E)\, \exp\left\{ \frac{i}{\hbar} \Big[\mathbf{p}\left(\mathbf{x} - \mathbf{x}' \right) - E(t - t') \Big] \right\} \tag{7.174}$$

yields straight-forwardly (7.174).