Chapter 21
Relativistic Quantum Fields

The quantized Maxwell field provided us already with an example of a relativistic quantum field theory. On the other hand, the description of relativistic charged particles requires Klein-Gordon fields for scalar particles and Dirac fields for fermions. Relativistic fields are apparently relevant for high energy physics. However, relativistic effects are also important in photon-matter interactions, spectroscopy, spin dynamics, and for the generation of brilliant photon beams from ultra-relativistic electrons in synchrotrons. Quasirelativistic effects from linear dispersion relations $E \propto \boldsymbol{p}$ in materials like Graphene and in Dirac semimetals have also reinvigorated the need to reconsider the role of Dirac and Weyl equations in materials science. In applications to materials with quasirelativistic dispersion relations c and m become effective velocity and mass parameters to describe cones or hyperboloids in regions of $(E, \boldsymbol{k})$ space.

We start our discussion of relativistic matter fields with the simpler Klein-Gordon equation and then move on to the more widely applicable Dirac equation. We will also discuss covariant quantization of photons, since this is more convenient for the calculation of basic scattering events than quantization in Coulomb gauge.

21.1 The Klein-Gordon equation

A limitation of the Schrödinger equation in the framework of ordinary quantum mechanics is its lack of covariance under Lorentz transformations[1]. On the other hand, we have encountered an example of a relativistic wave equation in Chapter 18,

[1]However, we will see that in the second quantized formalism in the Heisenberg and Dirac pictures, the time evolution of the field operators is given by Heisenberg equations of motion, and the corresponding time evolution of states in the Schrödinger and Dirac pictures is given by corresponding Schrödinger equations with relativistic Hamiltonians.

R. Dick, *Advanced Quantum Mechanics*, Graduate Texts in Physics,
DOI 10.1007/978-3-319-25675-7_21

viz. the inhomogeneous Maxwell equation

$$\partial_\mu \left(\partial^\mu A^\nu - \partial^\nu A^\mu\right) = -\mu_0 j^\nu.$$

This equation is manifestly covariant (or rather, form invariant) under Lorentz transformations because it is composed of quantities with simple tensorial transformation behavior under Lorentz transformations, and it relates a 4-vector $\partial_\mu F^{\mu\nu}$ to a 4-vector j^ν, such that the equation holds in this form in every inertial reference frame.

Another, simple reasoning to come up with a relativistic wave equation goes as follows. We know that the standard Schrödinger equation for a free massive particle arises from the non-relativistic energy-momentum dispersion relation $E = -cp_0 = \boldsymbol{p}^2/2m$ upon substitution of the classical energy-momentum vector through differential operators, $p_\mu \to -\mathrm{i}\hbar\partial_\mu$. Following the same procedure in the relativistic dispersion relation

$$-\frac{E^2}{c^2} + \boldsymbol{p}^2 + m^2c^2 = p^2 + m^2c^2 = 0$$

yields the free Klein-Gordon equation[2]

$$\left(\partial^2 - \frac{m^2c^2}{\hbar^2}\right)\phi(x) = \left(\Delta - \frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \frac{m^2c^2}{\hbar^2}\right)\phi(x) = 0. \tag{21.1}$$

Furthermore, the gauge principle or minimal coupling prescription $\partial_\mu \to D_\mu = \partial_\mu - \mathrm{i}(q/\hbar)A_\mu$ yields the coupling of the charged Klein-Gordon field to electromagnetic potentials,

$$\begin{aligned}\left[\left(\partial - \mathrm{i}\frac{q}{\hbar}A(x)\right)^2 - \frac{m^2c^2}{\hbar^2}\right]\phi(x) &= \left[\left(\nabla - \mathrm{i}\frac{q}{\hbar}\boldsymbol{A}(x)\right)^2\right.\\ &\left. - \frac{1}{c^2}\left(\frac{\partial}{\partial t} + \mathrm{i}\frac{q}{\hbar}\Phi(x)\right)^2 - \frac{m^2c^2}{\hbar^2}\right]\phi(x) = 0.\end{aligned} \tag{21.2}$$

Complex conjugation of equation (21.2) leads to the Klein-Gordon equation for a scalar field with charge $-q$. Therefore the *charge conjugate* Klein-Gordon field is simply gotten by complex conjugation,

$$\phi^c(x) = \phi^*(x). \tag{21.3}$$

The Klein-Gordon field is relevant in particle physics. E.g. π-mesons are described by Klein-Gordon fields as soon as their kinetic energy becomes

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[2] E. Schrödinger, Annalen Phys. 386, 109 (1926); W. Gordon, Z. Phys. 40, 117 (1926); O. Klein, Z. Phys. 41, 407 (1927).

comparable to their mass $mc^2 \simeq 140\,\text{MeV}$, when relativistic effects have to be taken into account. Another important application of the Klein-Gordon field is the Higgs field for electroweak symmetry breaking in the Standard Model of particle physics.

The Klein-Gordon field also provides a simple introduction into the relativistic quantum mechanics of charged particles. Therefore it is also useful as a preparation for the study of the Dirac field. We will focus in particular on the canonical quantization of freely evolving Klein-Gordon fields, since this describes Klein-Gordon operators in the practically relevant interaction picture representation. Conservation laws for full scalar quantum electrodynamics are discussed in Problems 21.6a and 21.7.

Mode expansion and quantization of the Klein-Gordon field

Fourier transformation of equation (21.1) yields the general solution of the free Klein-Gordon equation in $k = (\omega/c, \boldsymbol{k})$ space,

$$\begin{aligned}\phi(k) &= \phi(\boldsymbol{k},\omega) = \langle\boldsymbol{k}|\phi(\omega)\rangle \\ &= \sqrt{\frac{\pi}{\omega_{\boldsymbol{k}}}}\left[a(\boldsymbol{k})\delta(\omega-\omega_{\boldsymbol{k}}) + b^+(-\boldsymbol{k})\delta(\omega+\omega_{\boldsymbol{k}})\right], \end{aligned} \tag{21.4}$$

where $\omega_{\boldsymbol{k}}$ is just the k space expression for the relativistic dispersion relation,

$$\omega_{\boldsymbol{k}} = c\sqrt{\boldsymbol{k}^2 + (m^2c^2/\hbar^2)}.$$

Frequency-time Fourier transformation (5.12) yields

$$\langle\boldsymbol{k}|\phi(t)\rangle = \frac{1}{\sqrt{2\omega_{\boldsymbol{k}}}}\left[a(\boldsymbol{k})\exp(-\mathrm{i}\omega_{\boldsymbol{k}}t) + b^+(-\boldsymbol{k})\exp(\mathrm{i}\omega_{\boldsymbol{k}}t)\right]$$

and the general free Klein-Gordon wave function in $x = (ct, \boldsymbol{x})$ space is

$$\begin{aligned}\phi(x) = \langle\boldsymbol{x}|\phi(t)\rangle = \frac{1}{\sqrt{2\pi}^3}\int\frac{d^3\boldsymbol{k}}{\sqrt{2\omega_{\boldsymbol{k}}}}\Big(&a(\boldsymbol{k})\exp[\mathrm{i}(\boldsymbol{k}\cdot\boldsymbol{x}-\omega_{\boldsymbol{k}}t)] \\ &+ b^+(\boldsymbol{k})\exp[-\mathrm{i}(\boldsymbol{k}\cdot\boldsymbol{x}-\omega_{\boldsymbol{k}}t)]\Big).\end{aligned} \tag{21.5}$$

For the inversion of the Fourier transformation in the sense of solving for $a(\boldsymbol{k})$ and $b(\boldsymbol{k})$ we need equation (21.5) and

$$\begin{aligned}\dot{\phi}(\boldsymbol{x},t) = \frac{\mathrm{i}}{\sqrt{2\pi}^3}\int d^3\boldsymbol{k}\,\sqrt{\frac{\omega_{\boldsymbol{k}}}{2}}\Big(&-a(\boldsymbol{k})\exp[\mathrm{i}(\boldsymbol{k}\cdot\boldsymbol{x}-\omega_{\boldsymbol{k}}t)] \\ &+ b^+(\boldsymbol{k})\exp[-\mathrm{i}(\boldsymbol{k}\cdot\boldsymbol{x}-\omega_{\boldsymbol{k}}t)]\Big).\end{aligned}$$

Inversion of both equations yields

$$\begin{aligned} a(\boldsymbol{k}) &= \frac{1}{\sqrt{2\pi}^3}\int\frac{d^3\boldsymbol{x}}{\sqrt{2\omega_k}}\left(\omega_k\phi(\boldsymbol{x},t)+\mathrm{i}\dot{\phi}(\boldsymbol{x},t)\right)\exp[-\mathrm{i}(\boldsymbol{k}\cdot\boldsymbol{x}-\omega_k t)] \\ &= \frac{1}{\sqrt{2\pi}^3}\int\frac{d^3\boldsymbol{x}}{\sqrt{2\omega_k}}\exp[-\mathrm{i}(\boldsymbol{k}\cdot\boldsymbol{x}-\omega_k t)]\,\mathrm{i}\overleftrightarrow{\partial_t}\phi(\boldsymbol{x},t), \end{aligned} \tag{21.6}$$

$$\begin{aligned} b(\boldsymbol{k}) &= \frac{1}{\sqrt{2\pi}^3}\int\frac{d^3\boldsymbol{x}}{\sqrt{2\omega_k}}\left(\omega_k\phi^+(\boldsymbol{x},t)+\mathrm{i}\dot{\phi}^+(\boldsymbol{x},t)\right)\exp[-\mathrm{i}(\boldsymbol{k}\cdot\boldsymbol{x}-\omega_k t)] \\ &= \frac{1}{\sqrt{2\pi}^3}\int\frac{d^3\boldsymbol{x}}{\sqrt{2\omega_k}}\exp[-\mathrm{i}(\boldsymbol{k}\cdot\boldsymbol{x}-\omega_k t)]\,\mathrm{i}\overleftrightarrow{\partial_t}\phi^+(\boldsymbol{x},t). \end{aligned} \tag{21.7}$$

Here the alternating derivative is defined as

$$f\overleftrightarrow{\partial_t}g = f\frac{\partial g}{\partial t}-\frac{\partial f}{\partial t}g.$$

Substituting (21.6, 21.7) back into (21.5) and formal exchange of integrations yields

$$\phi(\boldsymbol{x},t) = \int d^3\boldsymbol{x}'\,\mathcal{K}(\boldsymbol{x}-\boldsymbol{x}',t-t')\,\overleftrightarrow{\partial_{t'}}\,\phi(\boldsymbol{x}',t') \tag{21.8}$$

with the time evolution kernel for free scalar fields,

$$\mathcal{K}(\boldsymbol{x},t) = \frac{1}{(2\pi)^3}\int\frac{d^3\boldsymbol{k}}{\omega_k}\exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x})\sin(\omega_k t). \tag{21.9}$$

This distribution satisfies the initial value problem

$$\left(\partial^2-\frac{m^2c^2}{\hbar^2}\right)\mathcal{K}(\boldsymbol{x},t)=0,\quad \mathcal{K}(\boldsymbol{x},0)=0,\quad \left.\frac{\partial}{\partial t}\mathcal{K}(\boldsymbol{x},t)\right|_{t=0}=\delta(\boldsymbol{x}).$$

For canonical quantization we need the Lagrange density for the complex Klein-Gordon field

$$\begin{aligned} \mathcal{L} &= \hbar\dot{\phi}^+\cdot\dot{\phi}-\hbar c^2\nabla\phi^+\cdot\nabla\phi-\frac{m^2c^4}{\hbar}\phi^+\cdot\phi \\ &= -\hbar c^2\partial\phi^+\cdot\partial\phi-\frac{m^2c^4}{\hbar}\phi^+\cdot\phi, \end{aligned} \tag{21.10}$$

or the real Klein-Gordon field

$$\mathcal{L} = \frac{\hbar}{2}\dot{\phi}\cdot\dot{\phi}-\frac{\hbar c^2}{2}\nabla\phi\cdot\nabla\phi-\frac{m^2c^4}{2\hbar}\phi^2 = -\frac{\hbar c^2}{2}(\partial\phi)^2-\frac{m^2c^4}{2\hbar}\phi^2. \tag{21.11}$$

In the following we will continue with the discussion of the complex Klein-Gordon field.

Canonical quantization proceeds from (21.10) without any problems. The conjugate momenta

$$\Pi_\phi = \frac{\partial\mathcal{L}}{\partial\dot{\phi}} = \hbar\dot{\phi}^+, \quad \Pi_{\phi^+} = \frac{\partial\mathcal{L}}{\partial\dot{\phi}^+} = \hbar\dot{\phi},$$

yield the canonical commutation relations in $\boldsymbol{x}$ space,

$$[\phi(\boldsymbol{x},t),\dot{\phi}^+(\boldsymbol{x}',t)] = \mathrm{i}\delta(\boldsymbol{x}-\boldsymbol{x}'), \quad [\phi^+(\boldsymbol{x},t),\dot{\phi}(\boldsymbol{x}',t)] = \mathrm{i}\delta(\boldsymbol{x}-\boldsymbol{x}'),$$
$$[\phi(\boldsymbol{x},t),\dot{\phi}(\boldsymbol{x}',t)] = 0, \quad [\phi(\boldsymbol{x},t),\phi(\boldsymbol{x}',t)] = 0, \quad [\phi(\boldsymbol{x},t),\phi^+(\boldsymbol{x}',t)] = 0,$$
$$[\dot{\phi}(\boldsymbol{x},t),\dot{\phi}(\boldsymbol{x}',t)] = 0, \quad [\dot{\phi}(\boldsymbol{x},t),\dot{\phi}^+(\boldsymbol{x}',t)] = 0,$$

and in $\boldsymbol{k}$ space,

$$[a(\boldsymbol{k}),a^+(\boldsymbol{k}')] = \delta(\boldsymbol{k}-\boldsymbol{k}'), \quad [a(\boldsymbol{k}),a(\boldsymbol{k}')] = 0, \quad [b(\boldsymbol{k}),b^+(\boldsymbol{k}')] = \delta(\boldsymbol{k}-\boldsymbol{k}'),$$
$$[b(\boldsymbol{k}),b(\boldsymbol{k}')] = 0, \quad [a(\boldsymbol{k}),b(\boldsymbol{k}')] = 0, \quad [a(\boldsymbol{k}),b^+(\boldsymbol{k}')] = 0.$$

The Lagrangian for interacting Klein-Gordon and Maxwell fields is

$$\mathcal{L} = -\frac{c^2}{\hbar}\left(\hbar\partial_\mu\phi^+ + \mathrm{i}q\phi^+\cdot A_\mu\right)\cdot(\hbar\partial^\mu\phi - \mathrm{i}qA^\mu\cdot\phi) - \frac{m^2c^4}{\hbar}\phi^+\cdot\phi$$
$$-\frac{1}{4\mu_0}F_{\mu\nu}F^{\mu\nu}. \tag{21.12}$$

The charge operator of the Klein-Gordon field

The Klein-Gordon Lagrangian (21.10) is invariant under phase transformations

$$\phi(x)\to\phi'(x) = \exp\left(\mathrm{i}\frac{q}{\hbar}\alpha\right)\phi(x), \quad \delta\phi(x) = \mathrm{i}\frac{q}{\hbar}\alpha\phi(x).$$

According to Section 16.2 this implies a local conservation law (16.13) for a conserved charge Q. After cancelling the superfluous factor α, the charge following from (16.14) is (after normal ordering of the integrand in $\boldsymbol{k}$ space, see the remarks following equations (18.40, 18.41))

$$Q = -\mathrm{i}\frac{q}{\hbar}\int d^3\boldsymbol{x}\left(\frac{\partial\mathcal{L}}{\partial\dot{\phi}}\cdot\phi - \phi^+\cdot\frac{\partial\mathcal{L}}{\partial\dot{\phi}^+}\right)$$
$$= -\mathrm{i}q\int d^3\boldsymbol{x}\left(\dot{\phi}^+(\boldsymbol{x},t)\cdot\phi(\boldsymbol{x},t) - \phi^+(\boldsymbol{x},t)\cdot\dot{\phi}(\boldsymbol{x},t)\right)$$
$$= q\int d^3\boldsymbol{k}\left(a^+(\boldsymbol{k})a(\boldsymbol{k}) - b^+(\boldsymbol{k})b(\boldsymbol{k})\right). \tag{21.13}$$

The charge density $\mathrm{i}q\phi^+ \overset{\leftrightarrow}{\partial_t} \phi$ is not positive definite, and therefore division of the charge density by q does not yield a probability density for the location of a particle, contrary to the Schrödinger field. Lack of a single particle interpretation is a generic property of relativistic fields which we had also encountered for the Maxwell field.

Hamiltonian and momentum operators for the Klein-Gordon field

The invariance of the Klein-Gordon Lagrangian (21.10) under constant translations

$$x^\mu \to x'^\mu = x^\mu + \delta x^\mu$$

implies a local conservation law (16.15) with corresponding conserved Hamilton and momentum operators (16.17). This yields the following expressions for energy and momentum of Klein-Gordon fields,

$$\mathcal{H} = -\Theta_0{}^0 = \hbar\dot{\phi}^+ \cdot \dot{\phi} + \hbar c^2 \nabla\phi^+ \cdot \nabla\phi + \frac{m^2c^4}{\hbar}\phi^+ \cdot \phi, \tag{21.14}$$

$$H = \int d^3\boldsymbol{x}\,\mathcal{H} = \int d^3\boldsymbol{k}\,\hbar\omega_{\boldsymbol{k}}\big(a^+(\boldsymbol{k})a(\boldsymbol{k}) + b^+(\boldsymbol{k})b(\boldsymbol{k})\big)\,, \tag{21.15}$$

$$\begin{aligned}\mathcal{P} &= \frac{1}{c}\boldsymbol{e}_i\Theta_i{}^0 = -\frac{\partial\mathcal{L}}{\partial\dot{\phi}}\cdot\nabla\phi - \nabla\phi^+\cdot\frac{\partial\mathcal{L}}{\partial\dot{\phi}^+} \\ &= -\hbar\dot{\phi}^+\cdot\nabla\phi - \hbar\nabla\phi^+\cdot\dot{\phi},\end{aligned} \tag{21.16}$$

$$\boldsymbol{P} = \int d^3\boldsymbol{x}\,\mathcal{P} = \int d^3\boldsymbol{k}\,\hbar\boldsymbol{k}\big(a^+(\boldsymbol{k})a(\boldsymbol{k}) + b^+(\boldsymbol{k})b(\boldsymbol{k})\big)\,. \tag{21.17}$$

The commutation relations and the charge operator (21.13), the Hamilton operator (21.15), and the momentum operators (21.17) imply that the operator $a^+(\boldsymbol{k})$ creates a particle of momentum $\hbar\boldsymbol{k}$, energy $\hbar\omega_{\boldsymbol{k}}$ and charge q, while $b^+(\boldsymbol{k})$ creates a particle of momentum $\hbar\boldsymbol{k}$, energy $\hbar\omega_{\boldsymbol{k}}$ and charge $-q$.

The operators (21.5) and $a(\boldsymbol{k},t) = a(\boldsymbol{k})\exp(-\mathrm{i}\omega_{\boldsymbol{k}}t)$, $a^+(\boldsymbol{k},t) = a^+(\boldsymbol{k})\exp(\mathrm{i}\omega_{\boldsymbol{k}}t)$ are the field operators in the Dirac picture, or the free field operators in the Heisenberg picture. They satisfy the Heisenberg evolution equations

$$\frac{\partial}{\partial t}a(\boldsymbol{k},t) = \frac{\mathrm{i}}{\hbar}[H, a(\boldsymbol{k},t)], \quad \frac{\partial}{\partial t}\phi(\boldsymbol{x},t) = \frac{\mathrm{i}}{\hbar}[H, \phi(\boldsymbol{x},t)],$$

with the free Hamiltonian (21.15). The corresponding integrals follow in the standard way,

$$a(\boldsymbol{k},t) = \exp\!\left(\frac{\mathrm{i}}{\hbar}Ht\right) a(\boldsymbol{k}) \exp\!\left(-\frac{\mathrm{i}}{\hbar}Ht\right),$$
$$\phi(\boldsymbol{x},t) = \exp\!\left(\frac{\mathrm{i}}{\hbar}Ht\right) \phi(\boldsymbol{x}) \exp\!\left(-\frac{\mathrm{i}}{\hbar}Ht\right),$$

etc. In the Schrödinger picture theory, this amounts to operators $a(\boldsymbol{k})$, $\phi(\boldsymbol{x})$, and time evolution of the states

$$\mathrm{i}\hbar\frac{d}{dt}|\Psi(t)\rangle = H|\Psi(t)\rangle$$

with the free Hamiltonian (21.15) for free states or a corresponding minimally coupled Hamiltonian which follows from (21.12) for interacting states, see Problem 21.5. This is the statement that we have Heisenberg and Schrödinger type evolution equations also in relativistic quantum field theory.

The Klein-Gordon equation also follows from the iterated Heisenberg equation,

$$\frac{\partial^2}{\partial t^2}\phi(\boldsymbol{x},t) = -\frac{1}{\hbar^2}[H,[H,\phi(\boldsymbol{x},t)]], \tag{21.18}$$

cf. (18.46) for photons.

Non-relativistic limit of the Klein-Gordon field

We have in the non-relativistic limit

$$\omega_{\boldsymbol{k}} = c\sqrt{\boldsymbol{k}^2 + \frac{m^2c^2}{\hbar^2}} \simeq \frac{mc^2}{\hbar} + \frac{\hbar\boldsymbol{k}^2}{2m},$$

and therefore in leading order also $1/\sqrt{2\omega_{\boldsymbol{k}}} \simeq \sqrt{\hbar/2mc^2}$.

Suppose that the $\boldsymbol{k}$-space amplitudes $a(\boldsymbol{k})$ and $b^+(\boldsymbol{k})$ are negligibly small unless $\hbar|\boldsymbol{k}| \ll mc$. In this case we can approximate equation (21.5) by

$$\phi(\boldsymbol{x},t) \simeq \frac{1}{\sqrt{2\pi}^3}\sqrt{\frac{\hbar}{2mc^2}}\int d^3\boldsymbol{k}\left[a(\boldsymbol{k})\exp\!\left(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x} - \mathrm{i}\frac{\hbar\boldsymbol{k}^2}{2m}t\right)\exp\!\left(-\mathrm{i}\frac{mc^2}{\hbar}t\right)\right.$$
$$\left. + \, b^+(\boldsymbol{k})\exp\!\left(-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x} + \mathrm{i}\frac{\hbar\boldsymbol{k}^2}{2m}t\right)\exp\!\left(\mathrm{i}\frac{mc^2}{\hbar}t\right)\right].$$

However, this expression automatically contains two fields

$$\psi(\boldsymbol{x},t) = \frac{1}{\sqrt{2\pi}^3}\int d^3\boldsymbol{k}\, a(\boldsymbol{k})\exp\!\left[\mathrm{i}\left(\boldsymbol{k}\cdot\boldsymbol{x} - \frac{\hbar\boldsymbol{k}^2}{2m}t\right)\right]$$

and

$$\varphi(\boldsymbol{x},t) = \frac{1}{\sqrt{2\pi}^3}\int d^3\boldsymbol{k}\, b(\boldsymbol{k}) \exp\left[\mathrm{i}\left(\boldsymbol{k}\cdot\boldsymbol{x} - \frac{\hbar\boldsymbol{k}^2}{2m}t\right)\right],$$

which satisfy the free Schrödinger equation, i.e. the complex Klein-Gordon field will reduce to a Schrödinger field $\psi(\boldsymbol{x},t)$ if the $\boldsymbol{k}$-space amplitudes also satisfy $|\langle a(\boldsymbol{k})\rangle| \gg |\langle b^+(\boldsymbol{k})\rangle|$.

Substitution of the remaining approximation

$$\phi(\boldsymbol{x},t) \simeq \sqrt{\frac{\hbar}{2mc^2}}\psi(\boldsymbol{x},t)\exp\left(-\mathrm{i}\frac{mc^2}{\hbar}t\right) \tag{21.19}$$

into the charge, current, energy and momentum densities of the Klein-Gordon field yields the corresponding expressions for the Schrödinger field,

$$\begin{aligned}
\varrho &= -\mathrm{i}q\left(\dot{\phi}^+\cdot\phi - \phi^+\cdot\dot{\phi}\right) \simeq q\psi^+\psi, \\
\boldsymbol{j} &= \mathrm{i}qc^2\left(\nabla\phi^+\cdot\phi - \phi^+\cdot\nabla\phi\right) \simeq q\frac{\hbar}{2\mathrm{i}m}\left(\psi^+\cdot\nabla\psi - \psi\cdot\nabla\psi^+\right), \\
\mathcal{H} &= \hbar\dot{\phi}^+\cdot\dot{\phi} + \hbar c^2\nabla\phi^+\cdot\nabla\phi + \frac{m^2c^4}{\hbar}\phi^+\cdot\phi \simeq \frac{\hbar^2}{2m}\nabla\psi^+\cdot\nabla\psi + mc^2\psi^+\cdot\psi, \\
\mathcal{P} &= -\hbar\dot{\phi}^+\cdot\nabla\phi - \hbar\nabla\phi^+\cdot\dot{\phi} \simeq \frac{\hbar}{2\mathrm{i}}\left(\psi^+\cdot\nabla\psi - \psi\cdot\nabla\psi^+\right) = \frac{m}{q}\boldsymbol{j}.
\end{aligned} \tag{21.20}$$

Furthermore, the free Klein-Gordon equation (21.1) becomes with

$$\frac{1}{c^2}\frac{\partial^2}{\partial t^2}\phi(\boldsymbol{x},t) \simeq \sqrt{\frac{\hbar}{2mc^2}}\exp\left(-\mathrm{i}\frac{mc^2}{\hbar}t\right)\left(-\frac{m^2c^2}{\hbar^2}\psi(\boldsymbol{x},t) - \mathrm{i}\frac{2m}{\hbar}\frac{\partial}{\partial t}\psi(\boldsymbol{x},t)\right)$$

the free Schrödinger equation

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

as it should, because we have already observed in the derivation of (21.19) that $\psi(\boldsymbol{x},t)$ satisfies the free Schrödinger equation.

For the non-relativistic limit of the real Klein-Gordon field we find

$$\phi(\boldsymbol{x},t) \simeq \sqrt{\frac{\hbar}{2mc^2}}\left[\psi(\boldsymbol{x},t)\exp\left(-\mathrm{i}\frac{mc^2}{\hbar}t\right) + \psi^+(\boldsymbol{x},t)\exp\left(\mathrm{i}\frac{mc^2}{\hbar}t\right)\right],$$

but we have to include first order time derivatives of $\psi(\boldsymbol{x},t)$ and $\psi^+(\boldsymbol{x},t)$ in the evaluation of $\mathcal{H}$ and $\boldsymbol{P}$, and then use the Schrödinger equation to find that remnant fast oscillation terms proportional to $\exp(\pm 2\mathrm{i}mc^2t/\hbar)$ reduce to boundary terms.

21.2 Klein's paradox

The commutation relations for the field operators $a(\boldsymbol{k})$ and $b^{+}(\boldsymbol{k})$ imply that the operator $\phi(\boldsymbol{x}, t)$ (21.5) describes both particles and anti-particles simultaneously, and therefore the Klein-Gordon equation cannot support a single particle interpretation. This is also obvious from the charge operator (21.13) and the corresponding lack of a conserved probability density for Klein-Gordon particles. Klein's paradox provides a particularly neat illustration of the failure of single particle interpretations of relativistic wave equations.

Klein observed that using relativistic quantum fields to describe a relativistic particle running against a potential step yields results for the transmission and reflection probabilities which are incompatible with a single particle interpretation[3]. This observation can be explained by pair creation in strong fields and the fact that relativistic fields describe both particles and anti-particles simultaneously. We will explain Klein's paradox for the Klein-Gordon field.

In the following we can neglect the y and z coordinates and deal only with the x and t coordinates. We are interested in a scalar particle of charge q scattered off a potential step of height $V > 0$. The step is located at $x = 0$, and can be implemented through an electrostatic potential $\Phi(x)$,

$$V(x) = q\Phi(x) = -cqA_0(x) = V\Theta(x). \tag{21.21}$$

Minimal coupling then yields the free Klein-Gordon equation for $x < 0$, and[4]

$$(\hbar\partial_t + \mathrm{i}V)^2\,\phi - \hbar^2c^2\partial_x^2\phi + m^2c^4\phi = 0 \tag{21.22}$$

for $x > 0$.

A monochromatic solution without any apparent left moving component for $x > 0$ is (after omission of an irrelevant constant prefactor)

$$\phi(x,t) = \begin{cases} [\exp(\mathrm{i}kx) + \beta\exp(-\mathrm{i}kx)]\exp(-\mathrm{i}\omega t), & x < 0 \\ \theta\exp[\mathrm{i}(\kappa x - \omega t)], & x > 0. \end{cases} \tag{21.23}$$

The frequency follows from the solution of the Klein-Gordon equation in the two domains,

$$\omega = c\sqrt{k^2 + \frac{m^2c^2}{\hbar^2}} = \frac{V}{\hbar} \pm c\sqrt{\kappa^2 + \frac{m^2c^2}{\hbar^2}}. \tag{21.24}$$

It has to be the same in both regions for continuity of the wave function at $x = 0$.

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[3]O. Klein, Z. Phys. 53, 157 (1929). Klein actually discussed reflection and transmission of relativistic spin 1/2 fermions which are described by the Dirac equation (21.38).

[4]We cannot try to discuss motion of particles of mass m in the presence of a potential by simply including a scalar potential term in the form $\left(\hbar^2\partial_t^2 - \hbar^2c^2\partial_x^2 + m^2c^4\right)\phi = \Theta(x)V^2\phi$ in the Klein-Gordon equation. This would correspond to a local mass $M(x)c^2 = \sqrt{m^2c^4 - \Theta(x)V^2}$ rather than to a local potential, and yield tachyons in $x > 0$ for $V^2 > m^2c^4$.

The sign in the last equation of (21.24) depends on the sign of $\hbar\omega - V$. We apparently have to use the minus sign if and only if $\hbar\omega - V < 0$. Note that in our solution we always have $\hbar\omega \geq mc^2$.

Solving for κ yields

$$\kappa = \pm\frac{1}{\hbar}\sqrt{\frac{(\hbar\omega - V)^2}{c^2} - m^2c^2} \in \mathbb{R}, \quad (\hbar\omega - V)^2 > m^2c^4, \tag{21.25}$$

$$\kappa = \frac{\mathrm{i}}{\hbar}\sqrt{m^2c^2 - \frac{(\hbar\omega - V)^2}{c^2}} \in \mathrm{i}\mathbb{R}_+, \quad (\hbar\omega - V)^2 < m^2c^4. \tag{21.26}$$

However, we have to be careful with the sign in (21.25). The group velocity in $x > 0$ for $\hbar\omega + mc^2 < V$ (i.e. for the negative sign in (21.24)) is

$$\frac{d\omega}{d\kappa} = -c\frac{\hbar\kappa}{\sqrt{\hbar^2\kappa^2 + m^2c^2}},$$

i.e. we have to take the *negative* root for κ for $V > \hbar\omega + mc^2$ to ensure positive group velocity in the region $x > 0$. We can collect the results for κ in the equations

$$\begin{aligned}
V < \hbar\omega - mc^2 : \quad & \kappa = \frac{1}{\hbar}\sqrt{\frac{(\hbar\omega-V)^2}{c^2} - m^2c^2} \in \mathbb{R}_+, \\
\hbar\omega - mc^2 < V < \hbar\omega + mc^2 : \quad & \kappa = \frac{\mathrm{i}}{\hbar}\sqrt{m^2c^2 - \frac{(\hbar\omega-V)^2}{c^2}} \in \mathrm{i}\mathbb{R}_+, \\
V > \hbar\omega + mc^2 : \quad & \kappa = -\frac{1}{\hbar}\sqrt{\frac{(\hbar\omega-V)^2}{c^2} - m^2c^2} \in \mathbb{R}_-.
\end{aligned}$$

The current density $j = \mathrm{i}qc^2(\partial_x\phi^+ \cdot \phi - \phi^+ \cdot \partial_x\phi)$ is

$$\begin{aligned}
j &= 2qc^2k\left(1 - |\beta|^2\right), && x < 0, \\
j &= 2qc^2\kappa|\theta|^2, && x > 0,\ \kappa \in \mathbb{R}, \\
j &= 0, && x > 0,\ \kappa \in \mathrm{i}\mathbb{R}.
\end{aligned} \tag{21.27}$$

Note that in $x > 0$ we have $j/q < 0$ if $V > \hbar\omega + mc^2$, in spite of the fact of positive group velocity in the region. Since charges q cannot move to the left in $x > 0$, this means that the negative value of j/q in $x > 0$ for $V > \hbar\omega + mc^2$ must correspond to right moving charges $-q$. We will see that this arises as a consequence of the generation of anti-particles near the potential step for $V > \hbar\omega + mc^2$.

The junction conditions

$$1 + \beta = \theta, \quad k(1 - \beta) = \kappa\theta \tag{21.28}$$

yield

$$\beta = \frac{k - \kappa}{k + \kappa}, \quad \theta = \frac{2k}{k + \kappa},$$

Table 21.1 Reflection and transmission for different relations between height V of the potential step and energy $\hbar\omega$ of the incident particle

$-\infty < V \le 0$	$\infty > \kappa \ge k$	$1 > R \ge 0$	$0 < T \le 1$
$0 \le V \le \hbar\omega - mc^2$	$k \ge \kappa \ge 0$	$0 \le R \le 1$	$1 \ge T \ge 0$
$\hbar\omega - mc^2 < V < \hbar\omega + mc^2$	$\kappa \in \mathrm{i}\mathbb{R}_+$	$R = 1$	$T = 0$
$\hbar\omega + mc^2 \le V \le 2\hbar\omega$	$0 \ge \kappa \ge -k$	$1 \le R \le \infty$	$0 \ge T \ge -\infty$
$2\hbar\omega \le V < \infty$	$-k \ge \kappa > -\infty$	$\infty \ge R > 1$	$-\infty \le T < 0$

and the corresponding reflection and transmission coefficients are

$$R = |\beta|^2 = \frac{k^2 + |\kappa|^2 - 2k\Re\kappa}{k^2 + |\kappa|^2 + 2k\Re\kappa}, \tag{21.29}$$

$$T = \frac{\Re\kappa}{k}|\theta|^2 = \frac{4k\Re\kappa}{k^2 + |\kappa|^2 + 2k\Re\kappa} = 1 - R. \tag{21.30}$$

The resulting behavior of the reflection coefficient is summarized in Table 21.1.

For an explanation of the unexpected result $R > 1$ for $V > \hbar\omega + mc^2 \ge 2mc^2$, recall that the solution for $V > \hbar\omega + mc^2$ in $x > 0$ has $\kappa < 0$. If we write the solution as

$$\phi(x,t) = \theta \exp[-\mathrm{i}(-\kappa x + \omega t)], \quad x > 0, \tag{21.31}$$

and compare with the anti-particle contribution to the free solution (21.5), we recognize the solution in the region $x > 0$ as an anti-particle solution with momentum $\hbar\kappa' = -\hbar\kappa > 0$ and energy

$$\overline{E}_p = -\hbar\omega < 0, \quad mc^2 - V \le \overline{E}_p \le -mc^2. \tag{21.32}$$

This is acceptable, because the anti-particle has charge $-q$ and therefore experiences a potential $U = -V$ in the region $x > 0$. Further support for this energy assignment for the anti-particles comes from the equality for the kinetic+rest energy of the anti-particles,

$$K_{\overline{p}} = c\sqrt{\hbar^2\kappa^2 + m^2c^2} = V - \hbar\omega, \quad mc^2 \le K_{\overline{p}} \le V - mc^2. \tag{21.33}$$

We expect $E_{\overline{p}} = K_{\overline{p}} - V$ at least in the non-relativistic limit for the anti-particles.

The anti-particles move to the right, $d(-\omega)/d(-\kappa) > 0$, and yield a negative particle current density $j/q \propto -q\kappa'/q = -\kappa' < 0$ due to the opposite charge. We therefore get $R > 1$ and $T < 0$ for $V - \hbar\omega > mc^2$ due to pair creation. The generated particles move to the left because they are repelled by the potential $V > mc^2 + \hbar\omega$. They add to the reflected particle in $x < 0$ to generate a formal reflection coefficient $R > 1$. The anti-particles move to the right because they can only move in the

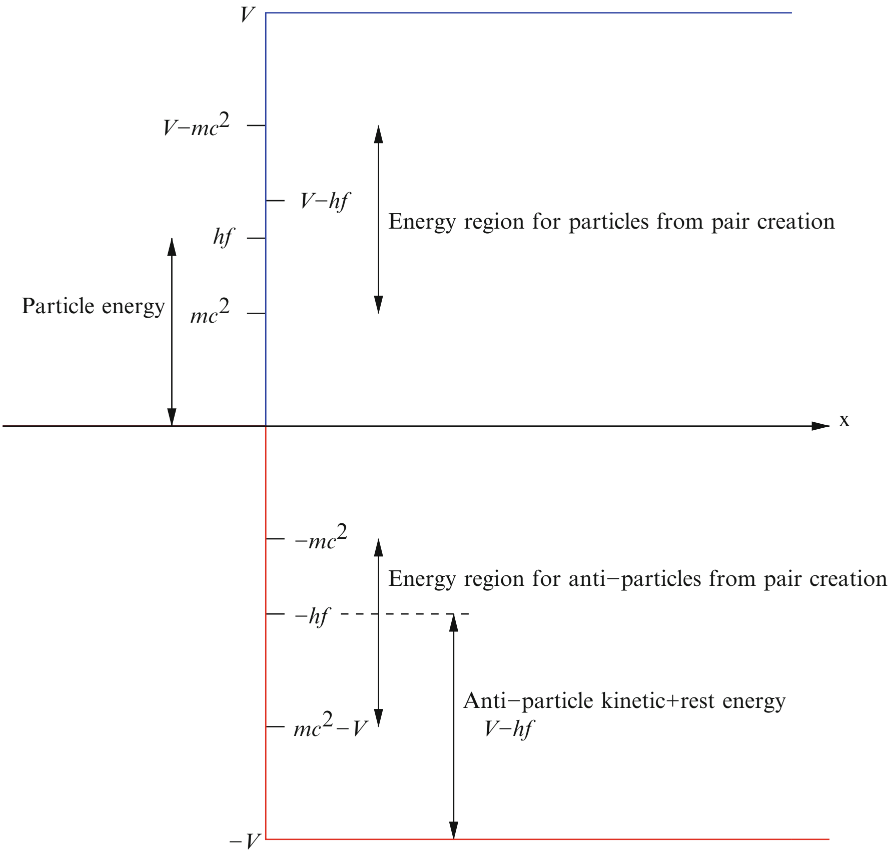

Fig. 21.1 Particles of charge q experience the potential V for $x > 0$, while anti-particles with charge $-q$ experience the potential $-V$. If the potential satisfies $V > 2mc^2$, it can produce particles with energy E_p, $mc^2 \le E_p = hf \le V - mc^2$, in the region $x < 0$ and anti-particles with energy $E_{\overline{p}} = -hf$, $mc^2 - V \le E_{\overline{p}} \le -mc^2$, in the region $x > 0$. This corresponds to a kinetic+rest energy $K_{\overline{p}} = V - hf$, $mc^2 \le K_{\overline{p}} \le V - mc^2$, see equation (21.33). Pair creation is most efficient for $hf = E_p = K_{\overline{p}} = -E_{\overline{p}} = V/2$

attractive potential $-V$ in $x > 0$. The movement of charges $-q$ to the right generates a negative apparent transmission coefficient $T = j_{x>0}/j_{in} < 0$.

Please note that the last two lines in Table 21.1 do *not* state that extremely large potentials $V \gg 2mc^2$ are less efficient for pair creation. They only state that a potential $V > 2mc^2$ is particularly efficient for generation of particle–anti-particle pairs with energies $E_p = K_{\overline{p}} = -E_{\overline{p}} = \hbar\omega = V/2$.

The conclusion in a nutshell is that if we wish to calculate scattering in the potential $V > 2mc^2$ for incident particles with energies in the pair creation region $mc^2 \le \hbar\omega \le V - mc^2$, then the ongoing pair creation will yield the seemingly paradoxical results $R > 1$ and $T = 1 - R < 0$, see Figure 21.1.

Please note that a more satisfactory discussion of energetics of the problem would also have to take into account the dynamics of the electromagnetic field $\Phi = V/q$, and then use the Hamiltonian density (21.132) of quantum electrodynamics with scalar matter. This would also imply an additional energy cost for separating the oppositely charged particles and anti-particles. The potential V would therefore decay due to pair creation until it satisfies the condition $V \leq 2mc^2$, when pair creation would seize and the standard single particle results $0 \leq T = 1 - R \leq 1$ apply for incident particles with any energy, or the potential would have to be maintained through an external energy source.

21.3 The Dirac equation

We have seen in equation (21.13) that the conserved charge of the complex Klein-Gordon field does not yield a conserved probability, and therefore has no single particle interpretation. This had motivated Paul Dirac in 1928 to propose a relativistic wave equation which is linear in the derivatives[5],

$$\mathrm{i}\hbar\gamma^{\mu}\partial_{\mu}\Psi(x) - mc\Psi(x) = 0. \tag{21.34}$$

Since the relativistic dispersion relation $p^2 + m^2c^2 = 0$ implies that the field Ψ should still satisfy the Klein-Gordon equation, equation (21.34) should imply the Klein-Gordon equation. Applying the operator $\mathrm{i}\hbar\gamma^{\mu}\partial_{\mu} + mc$ yields

$$-\hbar^2\gamma^{\mu}\gamma^{\nu}\partial_{\mu}\partial_{\nu}\Psi(x) - m^2c^2\Psi(x) = 0.$$

This is the Klein-Gordon equation if the coefficients γ^{μ} can be chosen to satisfy

$$\{\gamma^{\mu}, \gamma^{\nu}\} = -2\eta^{\mu\nu}. \tag{21.35}$$

In four dimensions, equation (21.35) has an up to equivalence transformations unique solution in terms of (4×4)-matrices (see Appendix G for the relevant proofs and for the construction of γ matrices in d spacetime dimensions).

The Dirac basis for γ matrices is

$$\gamma_0 = \begin{pmatrix} -\underline{1} & \underline{0} \\ \underline{0} & \underline{1} \end{pmatrix}, \quad \gamma_i = \begin{pmatrix} \underline{0} & \underline{\sigma}_i \\ -\underline{\sigma}_i & \underline{0} \end{pmatrix}, \tag{21.36}$$

where the (4×4)-matrices are expressed in terms of (2×2)-matrices. Another often used basis is the Weyl basis:

$$\gamma_0 = \begin{pmatrix} \underline{0} & \underline{1} \\ \underline{1} & \underline{0} \end{pmatrix}, \quad \gamma_i = \begin{pmatrix} \underline{0} & \underline{\sigma}_i \\ -\underline{\sigma}_i & \underline{0} \end{pmatrix}. \tag{21.37}$$

[5] P.A.M. Dirac, Proc. Roy. Soc. London A 117, 610 (1928). Dirac's relativistic wave equation was a great success, but like every relativistic wave equation, it also does not yield a single particle interpretation. It immediately proved itself by explaining the anomalous magnetic moment of the electron and the fine structure of spectral lines, and by predicting positrons.

The two bases are related by the orthogonal transformation

$$\gamma_W^\mu = \frac{1}{2}\begin{pmatrix} \underline{1} & \underline{1} \\ -\underline{1} & \underline{1} \end{pmatrix} \cdot \gamma_D^\mu \cdot \begin{pmatrix} \underline{1} & -\underline{1} \\ \underline{1} & \underline{1} \end{pmatrix},$$

$$\gamma_D^\mu = \frac{1}{2}\begin{pmatrix} \underline{1} & -\underline{1} \\ \underline{1} & \underline{1} \end{pmatrix} \cdot \gamma_W^\mu \cdot \begin{pmatrix} \underline{1} & \underline{1} \\ -\underline{1} & \underline{1} \end{pmatrix}.$$

The Dirac equation with minimal photon coupling

$$\gamma^\mu(\mathrm{i}\hbar\partial_\mu + qA_\mu)\Psi(x) - mc\Psi(x) = 0 \tag{21.38}$$

follows from the Lagrange density of quantum electrodynamics,

$$\mathcal{L} = c\overline{\Psi}\left[\gamma^\mu(\mathrm{i}\hbar\partial_\mu + qA_\mu) - mc\right]\Psi - \frac{1}{4\mu_0}F_{\mu\nu}F^{\mu\nu}, \quad \overline{\Psi} = \Psi^+\gamma^0. \tag{21.39}$$

The conserved current density for the phase invariance

$$\Psi' = \exp\!\left(\mathrm{i}\frac{q}{\hbar}\alpha\right)\Psi$$

is

$$j^\mu = cq\overline{\Psi}\gamma^\mu\Psi, \quad \varrho = j^0/c = q\Psi^+\Psi, \quad \boldsymbol{j} = cq\overline{\Psi}\boldsymbol{\gamma}\Psi. \tag{21.40}$$

Variation of (21.39) with respect to the vector potential shows that j^μ appears as the source term in Maxwell's equations,

$$\partial_\mu F^{\mu\nu} = -\mu_0 j^\nu.$$

Solutions of the free Dirac equation

We temporarily set $\hbar = 1$ and $c = 1$ for the construction of the general solution of the free Dirac equation.

Substitution of the Fourier *ansatz*

$$\Psi(x) = \int \frac{d^4p}{(2\pi)^2}\,\Psi(p)\exp(\mathrm{i}p\cdot x)$$

into (21.34) yields the equation

$$(\gamma^\mu p_\mu + m)\Psi(p) = 0. \tag{21.41}$$

We can use any representation of the γ matrices to find

$$\det(\gamma^\mu p_\mu + m) = (m^2 + p^2)^2 = (m^2 + \boldsymbol{p}^2 - E^2)^2 = (E^2(\boldsymbol{p}) - E^2)^2,$$

i.e. the solutions of (21.41) must have the form

$$\Psi(p) = \sqrt{\frac{\pi}{E(\boldsymbol{p})}}u(\boldsymbol{p})\delta(E - E(\boldsymbol{p})) + \sqrt{\frac{\pi}{E(\boldsymbol{p})}}v(-\boldsymbol{p})\delta(E + E(\boldsymbol{p})) \tag{21.42}$$

with $E(\boldsymbol{p}) = \sqrt{\boldsymbol{p}^2 + m^2}$ and

$$\left[\boldsymbol{\gamma}\cdot\boldsymbol{p} - \gamma^0 E(\boldsymbol{p}) + m\right]\cdot u(\boldsymbol{p}) = 0, \tag{21.43}$$

$$\left[\boldsymbol{\gamma}\cdot\boldsymbol{p} + \gamma^0 E(\boldsymbol{p}) + m\right]\cdot v(-\boldsymbol{p}) = 0. \tag{21.44}$$

The normalization factors in (21.42) are included for later convenience when we quantize the Dirac field.

To find the eigenspinors $u(\boldsymbol{p})$, $v(-\boldsymbol{p})$, we observe

$$(\gamma^\mu p_\mu + m)(m - \gamma^\mu p_\mu) = m^2 + p^2,$$

i.e. the columns $\zeta_{i+}(\boldsymbol{p})$ of the matrix $(m - \gamma^\mu p_\mu)_{E=E(\boldsymbol{p})}$ solve equation (21.43) while the columns $\zeta_{i-}(\boldsymbol{p})$ of the matrix $(m - \gamma^\mu p_\mu)_{E=-E(\boldsymbol{p})}$ solve equation (21.44). However, only two columns of each of the two matrices $\zeta_{i\pm}(\boldsymbol{p})$ are linearly independent.

We initially use a Dirac basis (21.36) for the γ matrices. A suitable basis for the general solution of the free Dirac equation is then given by the spin basis in the Dirac representation,

$$u(\boldsymbol{p}, \tfrac{1}{2}) = u_\uparrow(\boldsymbol{p}) = \frac{1}{\sqrt{E(\boldsymbol{p}) + m}}\zeta_{1+}(\boldsymbol{p}) = \frac{1}{\sqrt{E(\boldsymbol{p}) + m}}\begin{pmatrix} E(\boldsymbol{p}) + m \\ 0 \\ p_3 \\ p_+ \end{pmatrix}, \tag{21.45}$$

$$u(\boldsymbol{p}, -\tfrac{1}{2}) = u_\downarrow(\boldsymbol{p}) = \frac{1}{\sqrt{E(\boldsymbol{p}) + m}}\zeta_{2+}(\boldsymbol{p}) = \frac{1}{\sqrt{E(\boldsymbol{p}) + m}}\begin{pmatrix} 0 \\ E(\boldsymbol{p}) + m \\ p_- \\ -p_3 \end{pmatrix}, \tag{21.46}$$

$$v(-\boldsymbol{p}, -\tfrac{1}{2}) = v_\downarrow(-\boldsymbol{p}) = \frac{1}{\sqrt{E(\boldsymbol{p}) + m}} \zeta_{3-}(\boldsymbol{p})$$
$$= \frac{1}{\sqrt{E(\boldsymbol{p}) + m}} \begin{pmatrix} -p_3 \\ -p_+ \\ E(\boldsymbol{p}) + m \\ 0 \end{pmatrix}, \tag{21.47}$$

$$v(-\boldsymbol{p}, \tfrac{1}{2}) = v_\uparrow(-\boldsymbol{p}) = \frac{1}{\sqrt{E(\boldsymbol{p}) + m}} \zeta_{4-}(\boldsymbol{p})$$
$$= \frac{1}{\sqrt{E(\boldsymbol{p}) + m}} \begin{pmatrix} -p_- \\ p_3 \\ 0 \\ E(\boldsymbol{p}) + m \end{pmatrix}, \tag{21.48}$$

where $p_\pm = p_1 \pm \mathrm{i}p_2$ was used. The spin labels indicate that $u(\boldsymbol{p}, \pm\frac{1}{2})$ describes spin up or down particles, while $v(\boldsymbol{p}, \pm\frac{1}{2})$ describes spin up or down anti-particles.

It is also convenient to express the 4-spinors (21.45–21.48) in terms of the 2-spinors

$$\chi_\uparrow = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \chi_\downarrow = \begin{pmatrix} 0 \\ 1 \end{pmatrix},$$

in the form

$$u_\uparrow(\boldsymbol{p}) = \frac{1}{\sqrt{E(\boldsymbol{p}) + m}} \begin{pmatrix} (E(\boldsymbol{p}) + m)\chi_\uparrow \\ (\boldsymbol{p} \cdot \underline{\boldsymbol{\sigma}}) \cdot \chi_\uparrow \end{pmatrix},$$
$$u_\downarrow(\boldsymbol{p}) = \frac{1}{\sqrt{E(\boldsymbol{p}) + m}} \begin{pmatrix} (E(\boldsymbol{p}) + m)\chi_\downarrow \\ (\boldsymbol{p} \cdot \underline{\boldsymbol{\sigma}}) \cdot \chi_\downarrow \end{pmatrix},$$
$$v_\downarrow(\boldsymbol{p}) = \frac{1}{\sqrt{E(\boldsymbol{p}) + m}} \begin{pmatrix} (\boldsymbol{p} \cdot \underline{\boldsymbol{\sigma}}) \cdot \chi_\uparrow \\ (E(\boldsymbol{p}) + m)\chi_\uparrow \end{pmatrix},$$
$$v_\uparrow(\boldsymbol{p}) = \frac{1}{\sqrt{E(\boldsymbol{p}) + m}} \begin{pmatrix} (\boldsymbol{p} \cdot \underline{\boldsymbol{\sigma}}) \cdot \chi_\downarrow \\ (E(\boldsymbol{p}) + m)\chi_\downarrow \end{pmatrix}.$$

The general solution of the free Dirac equation then has the form

$$\Psi(x) = \frac{1}{\sqrt{2\pi}^3} \int \frac{d^3\boldsymbol{p}}{\sqrt{2E(\boldsymbol{p})}} \sum_{s \in \{\downarrow, \uparrow\}} \big[b_s(\boldsymbol{p}) u(\boldsymbol{p}, s) \exp(\mathrm{i}p \cdot x)$$
$$+ d_s^+(\boldsymbol{p}) v(\boldsymbol{p}, s) \exp(-\mathrm{i}p \cdot x) \big], \tag{21.49}$$

where $p^0 = E(\boldsymbol{p})$ is understood: $p \cdot x = \boldsymbol{p} \cdot \boldsymbol{x} - E(\boldsymbol{p})t$.

Calculations involving 4-spinors are often conveniently carried out with $\hbar = 1$ and $c = 1$, and restoration of the constants is usually only done in the final results from the requirement of correct units. For completeness I would also like to give the general solution of the free Dirac equation with the constants $\hbar$ and c restored. We can choose the basic spinors (21.45–21.48) to have units of square roots of energy, e.g.

$$u_{\uparrow}(\boldsymbol{k}) = \frac{1}{\sqrt{E(\boldsymbol{k}) + mc^2}} \begin{pmatrix} E(\boldsymbol{k}) + mc^2 \\ 0 \\ \hbar c k_3 \\ \hbar c k_+ \end{pmatrix}, \tag{21.50}$$

and the solution (21.49) is

$$\Psi(x) = \frac{1}{\sqrt{2\pi}^3} \int \frac{d^3\boldsymbol{k}}{\sqrt{2E(\boldsymbol{k})}} \sum_{s\in\{\downarrow,\uparrow\}} \big[b_s(\boldsymbol{k})u(\boldsymbol{k},s)\exp(\mathrm{i}k\cdot x) + d_s^+(\boldsymbol{k})v(\boldsymbol{k},s)\exp(-\mathrm{i}k\cdot x)\big] \tag{21.51}$$

with $k\cdot x \equiv \boldsymbol{k}\cdot\boldsymbol{x} - \omega(\boldsymbol{k})t$. In these conventions the Dirac field has the same dimensions length$^{-3/2}$ as the Schrödinger field. The free field $\Psi(x)$ also describes the freely evolving field operator $\Psi_D(x)$ in the interaction picture.

Some useful algebraic properties of the spinors (21.45–21.48) are frequently used in the calculations of cross sections and other observables,

$$u^+(\boldsymbol{k},s)\cdot u(\boldsymbol{k},s') = 2E(\boldsymbol{k})\delta_{ss'}, \quad v^+(\boldsymbol{k},s)\cdot v(\boldsymbol{k},s') = 2E(\boldsymbol{k})\delta_{ss'}, \tag{21.52}$$

$$u^+(\boldsymbol{k},s)\cdot v(-\boldsymbol{k},s') = 0, \quad \overline{u}(\boldsymbol{k},s)\cdot v(\boldsymbol{k},s') = 0, \tag{21.53}$$

$$\overline{u}(\boldsymbol{k},s)\cdot u(\boldsymbol{k},s') = 2mc^2\delta_{ss'}, \quad \overline{v}(\boldsymbol{k},s)\cdot v(\boldsymbol{k},s') = -2mc^2\delta_{ss'}, \tag{21.54}$$

$$\overline{u}(\boldsymbol{k},+)\cdot v(-\boldsymbol{k},-) = -2cp_3, \quad \overline{u}(\boldsymbol{k},+)\cdot v(-\boldsymbol{k},+) = -2cp_-, \tag{21.55}$$

$$\overline{u}(\boldsymbol{k},-)\cdot v(-\boldsymbol{k},-) = -2cp_+, \quad \overline{u}(\boldsymbol{k},-)\cdot v(-\boldsymbol{k},+) = 2cp_3. \tag{21.56}$$

The following equations contain 4×4 unit matrices $\underline{1}$ on the right hand sides,

$$\sum_s u(\boldsymbol{k},s)u^+(\boldsymbol{k},s) + \sum_s v(-\boldsymbol{k},s)v^+(-\boldsymbol{k},s) = 2E(\boldsymbol{k})\underline{1}, \tag{21.57}$$

$$\sum_s u(\boldsymbol{k},s)\overline{u}(\boldsymbol{k},s) = mc^2\underline{1} - c\gamma^\mu p_\mu\Big|_{cp^0=E(\boldsymbol{k})}, \tag{21.58}$$

$$\sum_s u(-\boldsymbol{k},s)\overline{u}(-\boldsymbol{k},s) = mc^2\underline{1} + c\gamma^\mu p_\mu\Big|_{cp^0=-E(\boldsymbol{k})}, \tag{21.59}$$

$$\sum_s v(\boldsymbol{k},s)\overline{v}(\boldsymbol{k},s) = -mc^2\underline{1} - c\gamma^\mu p_\mu\Big|_{cp^0=E(\boldsymbol{k})}, \tag{21.60}$$

$$\sum_s v(-\boldsymbol{k},s)\overline{v}(-\boldsymbol{k},s) = -mc^2\underline{1} + c\gamma^\mu p_\mu\Big|_{cp^0=-E(\boldsymbol{k})}. \tag{21.61}$$

It is actually clumsy to write down unit matrices when their presence is clear from the context, and the action e.g. of the scalar mc^2 on a 4-spinor Ψ has the same effect as the matrix $mc^2\underline{1}$. Therefore we will usually adopt the practice of not writing down 4×4 unit matrices explicitly.

Equations (21.52) and (21.53) are used e.g. in the inversion of the Fourier representation (21.51),

$$b_s(\boldsymbol{k}) = \frac{1}{\sqrt{2\pi}^3}\int\frac{d^3\boldsymbol{x}}{\sqrt{2E(\boldsymbol{k})}}\,\exp(-\mathrm{i}k\cdot x)u^+(\boldsymbol{k},s)\cdot\Psi(x), \tag{21.62}$$

$$d_s(\boldsymbol{k}) = \frac{1}{\sqrt{2\pi}^3}\int\frac{d^3\boldsymbol{x}}{\sqrt{2E(\boldsymbol{k})}}\,\exp(-\mathrm{i}k\cdot x)\Psi^+(x)\cdot v(\boldsymbol{k},s). \tag{21.63}$$

Substituting these equations back into (21.51) yields

$$\Psi(\boldsymbol{x},t) = \int d^3\boldsymbol{x}'\,\mathcal{W}(\boldsymbol{x}-\boldsymbol{x}',t-t')\cdot\Psi(\boldsymbol{x}',t') \tag{21.64}$$

with the time evolution kernel

$$\begin{aligned}\mathcal{W}(\boldsymbol{x},t) &= \frac{1}{(2\pi)^3}\int\frac{d^3\boldsymbol{k}}{2E(\boldsymbol{k})}\,\exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x})\sum_s[u(\boldsymbol{k},s)u^+(\boldsymbol{k},s)\exp(-\mathrm{i}\omega(\boldsymbol{k})t)\\ &\quad + v(-\boldsymbol{k},s)v^+(-\boldsymbol{k},s)\exp(\mathrm{i}\omega(\boldsymbol{k})t)]\\ &= \frac{1}{(2\pi)^3}\int\frac{d^3\boldsymbol{k}}{E(\boldsymbol{k})}\,\exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x})[E(\boldsymbol{k})\cos(\omega(\boldsymbol{k})t)\\ &\quad + \mathrm{i}c(\hbar\boldsymbol{\gamma}\cdot\boldsymbol{k} - mc)\gamma^0\sin(\omega(\boldsymbol{k})t)].\end{aligned} \tag{21.65}$$

This satisfies the initial value problem

$$(\mathrm{i}\hbar\gamma^\mu\partial_\mu - mc)\mathcal{W}(\boldsymbol{x},t) = 0, \quad \mathcal{W}(\boldsymbol{x},0) = \delta(\boldsymbol{x}). \tag{21.66}$$

It is related to the time evolution kernel (21.9) of the Klein-Gordon field through

$$\mathrm{i}\mathcal{W}(\boldsymbol{x},t)\gamma^0 = c\left(\mathrm{i}\gamma\cdot\partial + \frac{mc}{\hbar}\right)\mathcal{K}(\boldsymbol{x},t). \tag{21.67}$$

It is sometimes useful to express equation (21.49) and the corresponding equation in $\boldsymbol{k}$ space in bra-ket notation, similar to equations (18.24, 18.25) for the Maxwell field. With the definitions

$$b_{+,s}(\boldsymbol{k}) = b_s(\boldsymbol{k}), \quad b_{-,s}(\boldsymbol{k}) = d_s^+(-\boldsymbol{k}),$$

$$u_{+,s}(\boldsymbol{k}) = u_s(\boldsymbol{k}), \quad u_{-,s}(\boldsymbol{k}) = v_s(-\boldsymbol{k}),$$

we can write the free Dirac field in the forms

$$\langle \boldsymbol{k}, \sigma, s|\Psi(t)\rangle = b_{\sigma,s}(\boldsymbol{k}) \exp[-\mathrm{i}\sigma\omega(\boldsymbol{k})t] \tag{21.68}$$

and

$$\langle \boldsymbol{x}, a|\Psi(t)\rangle = \int \frac{d^3\boldsymbol{k}}{\sqrt{2\pi}^3} \sum_{\sigma\in\{+,-\}} \sum_{s\in\{\uparrow,\downarrow\}} \frac{b_{\sigma,s}(\boldsymbol{k})u^a_{\sigma,s}(\boldsymbol{k})}{\sqrt{2\hbar\omega(\boldsymbol{k})}} \exp[\mathrm{i}(\boldsymbol{k}\cdot\boldsymbol{x} - \sigma\omega(\boldsymbol{k})t)],$$

where $a \in \{1, \ldots 4\}$ is a Dirac spinor index, $\sigma \in \{+, -\}$ labels particles $(+)$ or antiparticles $(-)$, and s is the spin label. The equations (21.52) and the first equation in (21.53) are

$$u^+_{\sigma,s}(\boldsymbol{k}) \cdot u_{\sigma',s'}(\boldsymbol{k}) = 2\hbar\omega(\boldsymbol{k})\delta_{\sigma,\sigma'}\delta_{s,s'}. \tag{21.69}$$

Equation (21.54) is

$$\overline{u}_{\sigma,s}(\boldsymbol{k}) \cdot u_{\sigma,s'}(\boldsymbol{k}) = 2mc^2\sigma\delta_{ss'}, \tag{21.70}$$

and equation (21.57) is

$$\sum_{\sigma,s} u_{\sigma,s}(\boldsymbol{k})u^+_{\sigma,s}(\boldsymbol{k}) = 2\hbar\omega(\boldsymbol{k})\underline{1}. \tag{21.71}$$

The $\boldsymbol{x}$ representations of the spinor momentum eigenstates are

$$\langle \boldsymbol{x}, a|\boldsymbol{k}, \sigma, s\rangle = \frac{\exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x})}{4\pi\sqrt{\pi\hbar\omega(\boldsymbol{k})}} u^a_{\sigma,s}(\boldsymbol{k}), \tag{21.72}$$

and using equations (21.69, 21.71) we can easily verify the relations

$$\langle \boldsymbol{k}, \sigma, s|\boldsymbol{k}', \sigma', s'\rangle = \delta_{\sigma,\sigma'}\delta_{s,s'}\delta(\boldsymbol{k} - \boldsymbol{k}'), \quad \langle \boldsymbol{x}, a|\boldsymbol{x}', a'\rangle = \delta_{a,a'}\delta(\boldsymbol{x} - \boldsymbol{x}'). \tag{21.73}$$

Charge operators and quantization of the Dirac field

We can apply the results from Section 16.2 to calculate the energy and momentum operator for the Dirac field. The free Dirac Lagrangian

$$\mathcal{L} = c\overline{\Psi}\left(\mathrm{i}\hbar\gamma^\mu\partial_\mu - mc\right)\Psi \tag{21.74}$$

yields the positive definite normal ordered Hamiltonian

$$H = \int d^3\boldsymbol{x}\, c\overline{\Psi}(\boldsymbol{x}, t)\,(mc - \mathrm{i}\hbar\boldsymbol{\gamma}\cdot\nabla)\,\Psi(\boldsymbol{x}, t)$$

$$= \int d^3\boldsymbol{k}\,\hbar\omega(\boldsymbol{k}) \sum_{s\in\{\downarrow,\uparrow\}} \left[b_s^+(\boldsymbol{k})b_s(\boldsymbol{k}) + d_s^+(\boldsymbol{k})d_s(\boldsymbol{k})\right], \tag{21.75}$$

but only if we assume anti-commutation properties of the d_s and d_s^+ operators.

The normal ordered momentum operator is then

$$\begin{aligned}\boldsymbol{P} &= \int d^3\boldsymbol{x}\,\Psi^+(\boldsymbol{x},t)\frac{\hbar}{\mathrm{i}}\nabla\Psi(\boldsymbol{x},t)\\ &= \int d^3\boldsymbol{k}\,\hbar\boldsymbol{k} \sum_{s\in\{\downarrow,\uparrow\}} \left[b_s^+(\boldsymbol{k})b_s(\boldsymbol{k}) + d_s^+(\boldsymbol{k})d_s(\boldsymbol{k})\right].\end{aligned} \tag{21.76}$$

The electromagnetic current density (21.40) yields the charge operator

$$\begin{aligned}Q &= q\int d^3\boldsymbol{x}\,\Psi^+(\boldsymbol{x},t)\Psi(\boldsymbol{x},t)\\ &= q\int d^3\boldsymbol{k} \sum_{s\in\{\downarrow,\uparrow\}} \left[b_s^+(\boldsymbol{k})b_s(\boldsymbol{k}) - d_s^+(\boldsymbol{k})d_s(\boldsymbol{k})\right].\end{aligned} \tag{21.77}$$

The normalization in equation (21.51) has been chosen such that the quantization condition

$$\{\Psi_\alpha(\boldsymbol{x},t), \Psi_\beta{}^+(\boldsymbol{x}',t)\} = \delta_{\alpha\beta}\delta(\boldsymbol{x}-\boldsymbol{x}')$$

for the components of $\Psi(x)$ yields

$$\{b(\boldsymbol{k},s), b^+(\boldsymbol{k}',s')\} = \delta_{ss'}\delta(\boldsymbol{k}-\boldsymbol{k}'), \quad \{d(\boldsymbol{k},s), d^+(\boldsymbol{k}',s')\} = \delta_{ss'}\delta(\boldsymbol{k}-\boldsymbol{k}'),$$

with the other anti-commutators vanishing. The equations (21.75–21.77) then imply that the operator $b^+(\boldsymbol{k},s)$ creates a fermion of mass m, momentum $\hbar\boldsymbol{k}$ and charge q, while $d^+(\boldsymbol{k},s)$ creates a particle with the same mass and momentum, but opposite charge $-q$.

For an explanation of the spin labels of the spinors $u(\boldsymbol{k},\pm\frac{1}{2})$, we notice that the spin operators corresponding to the rotation generators

$$M_i = -\mathrm{i}L_i = \frac{1}{2}\epsilon_{ijk}M_{jk}$$

are both in the Dirac and in the Weyl representation given by

$$S_i = \frac{\hbar}{2}\epsilon_{ijk}S_{jk} = \frac{\mathrm{i}\hbar}{4}\epsilon_{ijk}\gamma_j\gamma_k = \frac{\hbar}{2}\begin{pmatrix}\underline{\sigma}_i & 0\\ 0 & \underline{\sigma}_i\end{pmatrix}, \tag{21.78}$$

see Appendix H for an explanation of generators of Lorentz boosts and rotations for Dirac spinors.

Equation (21.78) implies that the rest frame spinors $u(\mathbf{0}, \pm\frac{1}{2})$ transform under rotations around the z axis as spinors with z-component of spin $\hbar s = \pm\hbar/2$.

For an explanation of the spin labels of the spinors $v(\boldsymbol{p}, \pm\frac{1}{2})$, we have to look at charge conjugation. Both in the Dirac and the Weyl representation of γ matrices we have

$$\gamma_\mu^* = \gamma_2\gamma_\mu\gamma_2.$$

Therefore complex conjugation of the Dirac equation

$$[\mathrm{i}\gamma^\mu\partial_\mu + q\gamma^\mu A_\mu(x) - m]\Psi(x) = 0,$$

followed by multiplication with $\mathrm{i}\gamma_2$ from the left yields

$$[\mathrm{i}\gamma^\mu\partial_\mu - q\gamma^\mu A_\mu(x) - m]\Psi^c(x) = 0$$

with the charge conjugate field

$$\Psi^c(x) = \mathrm{i}\gamma_2\Psi^*(x). \tag{21.79}$$

In particular, we have

$$v^c(\boldsymbol{k}, \tfrac{1}{2}) = \mathrm{i}\gamma_2 v^*(\boldsymbol{k}, \tfrac{1}{2}) = u(\boldsymbol{k}, \tfrac{1}{2})$$

and

$$v^c(\boldsymbol{k}, -\tfrac{1}{2}) = \mathrm{i}\gamma_2 v^*(\boldsymbol{k}, -\tfrac{1}{2}) = -u(\boldsymbol{k}, -\tfrac{1}{2}),$$

i.e. the negative energy spinors for charge q, momentum $\hbar\boldsymbol{k}$ and spin projection $\hbar s$ correspond to positive energy spinors for charge $-q$, momentum $\hbar\boldsymbol{k}$ and spin projection $\hbar s$.

21.4 The energy-momentum tensor for quantum electrodynamics

We use the symmetrized form of the QED Lagrangian (21.39),

$$\mathcal{L} = c\overline{\Psi}\left[\gamma^\mu\left(\frac{\mathrm{i}\hbar}{2}\overset{\leftrightarrow}{\partial}_\mu + qA_\mu\right) - mc\right]\Psi - \frac{1}{4\mu_0}F_{\mu\nu}F^{\mu\nu}. \tag{21.80}$$

This yields according to (16.16) a conserved energy-momentum tensor

$$\begin{aligned}\Theta_\mu{}^\nu &= \eta_\mu{}^\nu\mathcal{L} - \partial_\mu\overline{\Psi}\frac{\partial\mathcal{L}}{\partial(\partial_\nu\overline{\Psi})} - \partial_\mu\Psi\frac{\partial\mathcal{L}}{\partial(\partial_\nu\Psi)} - \partial_\mu A_\lambda\frac{\partial\mathcal{L}}{\partial(\partial_\nu A_\lambda)}\\ &= \eta_\mu{}^\nu\left(c\overline{\Psi}\left[\gamma^\lambda\left(\frac{i\hbar}{2}\overset{\leftrightarrow}{\partial}_\lambda + qA_\lambda\right) - mc\right]\Psi - \frac{1}{4\mu_0}F_{\kappa\lambda}F^{\kappa\lambda}\right)\\ &\quad -\frac{i\hbar}{2}c\overline{\Psi}\gamma^\nu\overset{\leftrightarrow}{\partial}_\mu\Psi + \frac{1}{\mu_0}\partial_\mu A_\lambda F^{\nu\lambda}.\end{aligned}$$

According to the results of Section 16.2, this yields on-shell conserved charges, i.e. we can use the equations of motion to simplify this expression. The Dirac equation then implies

$$\Theta_\mu{}^\nu = -\frac{i\hbar}{2}c\overline{\Psi}\gamma^\nu\overset{\leftrightarrow}{\partial}_\mu\Psi + \frac{1}{\mu_0}\partial_\mu A_\lambda F^{\nu\lambda} - \frac{1}{4\mu_0}\eta_\mu{}^\nu F_{\kappa\lambda}F^{\kappa\lambda}.$$

We can also add the identically conserved improvement term

$$\begin{aligned}-\frac{1}{\mu_0}\partial_\lambda\left(A_\mu F^{\nu\lambda}\right) &= -\frac{1}{\mu_0}\partial_\lambda A_\mu F^{\nu\lambda} - \frac{1}{\mu_0}A_\mu\partial_\lambda F^{\nu\lambda}\\ &= -\frac{1}{\mu_0}\partial_\lambda A_\mu F^{\nu\lambda} - qcA_\mu\overline{\Psi}\gamma^\nu\Psi,\end{aligned}$$

where Maxwell's equations $\partial_\mu F^{\mu\nu} = -\mu_0 qc\overline{\Psi}\gamma^\nu\Psi$ have been used. This yields the gauge invariant tensor

$$\begin{aligned}t_\mu{}^\nu &= \Theta_\mu{}^\nu - \frac{1}{\mu_0}\partial_\lambda\left(A_\mu F^{\nu\lambda}\right)\\ &= -\frac{i\hbar}{2}c\overline{\Psi}\gamma^\nu\overset{\leftrightarrow}{\partial}_\mu\Psi - qc\overline{\Psi}\gamma^\nu A_\mu\Psi + \frac{1}{\mu_0}F_{\mu\lambda}F^{\nu\lambda} - \eta_\mu{}^\nu\frac{1}{4\mu_0}F_{\kappa\lambda}F^{\kappa\lambda}. \quad (21.81)\end{aligned}$$

However, we can go one step further and replace $t_\mu{}^\nu$ with a symmetric energy-momentum tensor. The divergence of the spinor term in $t_\mu{}^\nu$ is

$$\partial_\nu\left(\frac{i\hbar}{2}\overline{\Psi}\gamma^\nu\overset{\leftrightarrow}{\partial}_\mu\Psi + q\overline{\Psi}\gamma^\nu A_\mu\Psi\right) = -q\overline{\Psi}F_{\mu\nu}\gamma^\nu\Psi, \quad (21.82)$$

where again the Dirac equation was used.

The symmetrization of $t_\mu{}^\nu$ also involves the commutators of γ matrices,

$$S_{\mu\nu} = \frac{i}{4}[\gamma_\mu, \gamma_\nu] = \gamma_0\cdot S^+_{\mu\nu}\cdot\gamma_0. \quad (21.83)$$

Since we can write a product always as a sum of an anti-commutator and a commutator, we have

$$\gamma_\mu\cdot\gamma_\nu = -\eta_{\mu\nu} - 2iS_{\mu\nu}, \quad (21.84)$$

and the commutators also satisfy[6]

$$\eta_{\mu\alpha}\gamma_\beta - \eta_{\mu\beta}\gamma_\alpha + \mathrm{i}[S_{\alpha\beta}, \gamma_\mu] = 0. \tag{21.85}$$

Equations (21.83–21.85) together with

$$\begin{aligned}\hbar^2\partial^2\Psi &= \mathrm{i}\hbar\gamma^\mu\partial_\mu\left(mc\Psi - q\gamma^\nu A_\nu\Psi\right)\\ &= \mathrm{i}\hbar q\left[\partial_\mu\left(A^\mu\Psi\right) + 2\mathrm{i}S^{\mu\nu}\partial_\mu\left(A_\nu\Psi\right)\right] + mc\left[mc\Psi - q\gamma^\nu A_\nu\Psi\right]\end{aligned}$$

imply also

$$\partial_\nu\left(\frac{\mathrm{i}\hbar}{2}\overline{\Psi}\gamma_\mu \overset{\leftrightarrow}{\partial^\nu}\Psi + q\overline{\Psi}\gamma_\mu A^\nu\Psi\right) = -q\overline{\Psi}F_{\mu\nu}\gamma^\nu\Psi. \tag{21.86}$$

Therefore the local conservation law $\partial_\nu T_\mu{}^\nu = 0$ also holds for the symmetrized energy-momentum tensor

$$\begin{aligned}T_\mu{}^\nu = &-\frac{c}{2}\overline{\Psi}\left[\frac{\mathrm{i}\hbar}{2}\gamma^\nu \overset{\leftrightarrow}{\partial_\mu} + \frac{\mathrm{i}\hbar}{2}\gamma_\mu \overset{\leftrightarrow}{\partial^\nu} + q\gamma^\nu A_\mu + q\gamma_\mu A^\nu\right]\Psi\\ &+ \frac{1}{\mu_0}F_{\mu\lambda}F^{\nu\lambda} - \eta_\mu{}^\nu\frac{1}{4\mu_0}F_{\kappa\lambda}F^{\kappa\lambda}.\end{aligned} \tag{21.87}$$

This yields in particular the Hamiltonian density

$$\begin{aligned}\mathcal{H} = -T_0{}^0 &= c\Psi^+\left[\frac{\mathrm{i}\hbar}{2}\overset{\leftrightarrow}{\partial_0} + qA_0\right]\Psi + \frac{\epsilon_0}{2}\boldsymbol{E}^2 + \frac{1}{2\mu_0}\boldsymbol{B}^2\\ &= c\overline{\Psi}\left[mc - \frac{\mathrm{i}\hbar}{2}\boldsymbol{\gamma}\cdot\overset{\leftrightarrow}{\nabla} - q\boldsymbol{\gamma}\cdot\boldsymbol{A}\right]\Psi + \frac{\epsilon_0}{2}\boldsymbol{E}^2 + \frac{1}{2\mu_0}\boldsymbol{B}^2,\end{aligned} \tag{21.88}$$

and the momentum density with components $\mathcal{P}_i = T_i{}^0/c$,

$$\mathcal{P} = \frac{1}{2}\Psi^+\left[\frac{\hbar}{2\mathrm{i}}\overset{\leftrightarrow}{\nabla} - q\boldsymbol{A}\right]\Psi + \frac{1}{2}\overline{\Psi}\boldsymbol{\gamma}\left[\frac{\mathrm{i}\hbar}{2}\overset{\leftrightarrow}{\partial_0} + qA_0\right]\Psi + \epsilon_0\boldsymbol{E}\times\boldsymbol{B}. \tag{21.89}$$

Elimination of the time derivatives using the Dirac equation yields

$$\mathcal{P} = \Psi^+\left[\frac{\hbar}{2\mathrm{i}}\overset{\leftrightarrow}{\nabla} - q\boldsymbol{A}\right]\Psi + \epsilon_0\boldsymbol{E}\times\boldsymbol{B} + \frac{1}{2}\nabla\times(\Psi^+\cdot\boldsymbol{S}\cdot\Psi). \tag{21.90}$$

[6]The commutators $S_{\mu\nu}$ provide the spinor representation of the generators of Lorentz transformations. Furthermore, equation (21.85) is the invariance of the γ matrices under Lorentz transformations, see Appendix H.

The spin contribution $\mathcal{P}_S = \nabla \times (\Psi^+ \cdot \boldsymbol{S} \cdot \Psi)/2$ with the vector of 4×4 spin matrices $\boldsymbol{S} = \mathrm{i}\hbar\boldsymbol{\gamma} \times \boldsymbol{\gamma}/4$ (21.78) appears here as an additional contribution compared to the orbital momentum density $\mathcal{P}_O = \mathcal{P} - \mathcal{P}_S$ that follows directly from the tensor (21.81). The spin term in the momentum density (21.90) generates the spin contribution in the total angular momentum density $\mathcal{J} = \boldsymbol{x} \times \mathcal{P} = \mathcal{M} + \mathcal{S}$ from $\mathcal{S} = \boldsymbol{x} \times \mathcal{P}_S \to \Psi^+ \cdot \boldsymbol{S} \cdot \Psi$ if the symmetric energy-momentum tensor is used in the calculation of angular momentum. This is explained in Problem 21.16c, see in particular equations (21.147–21.150).

Energy and momentum in QED in Coulomb gauge

In materials science it is convenient to explicitly disentangle the contributions from Coulomb and photon terms in Coulomb gauge $\nabla \cdot \boldsymbol{A} = 0$. We split the electric field components in Coulomb gauge according to

$$\boldsymbol{E}_\parallel = -\nabla\Phi, \quad \boldsymbol{E}_\perp = -\frac{\partial \boldsymbol{A}}{\partial t}. \tag{21.91}$$

The equation for the electrostatic potential decouples from the vector potential in Coulomb gauge,

$$\Delta\Phi = -\frac{q}{\epsilon_0}\Psi^+\Psi,$$

and is solved by

$$\Phi(\boldsymbol{x}, t) = \frac{q}{4\pi\epsilon_0}\int d^3\boldsymbol{x}' \,\frac{1}{|\boldsymbol{x} - \boldsymbol{x}'|}\Psi^+(\boldsymbol{x}', t)\Psi(\boldsymbol{x}', t).$$

Furthermore, the two components (21.91) of the electric field are orthogonal in Coulomb gauge,

$$\begin{aligned}\int d^3\boldsymbol{x}\, \boldsymbol{E}_\parallel(\boldsymbol{x}, t) \cdot \boldsymbol{E}_\perp(\boldsymbol{x}, t) &= \int d^3\boldsymbol{k}\, \boldsymbol{E}_\parallel(\boldsymbol{k}, t) \cdot \boldsymbol{E}_\perp(-\boldsymbol{k}, t) \\ &= -\int d^3\boldsymbol{x}\, \Phi(\boldsymbol{x}, t)\frac{\partial}{\partial t}\nabla \cdot \boldsymbol{A}(\boldsymbol{x}, t) = 0,\end{aligned} \tag{21.92}$$

and the contribution from $\boldsymbol{E}_\parallel$ to the Hamiltonian is

$$\begin{aligned}H_C &= \frac{\epsilon_0}{2}\int d^3\boldsymbol{x}\, \boldsymbol{E}_\parallel^2(\boldsymbol{x}, t) = -\frac{\epsilon_0}{2}\int d^3\boldsymbol{x}\, \Phi(\boldsymbol{x}, t)\Delta\Phi(\boldsymbol{x}, t) \\ &= \frac{1}{2}\int d^3\boldsymbol{x}\, \Phi(\boldsymbol{x}, t)\varrho(\boldsymbol{x}, t)\end{aligned}$$

$$= q^2 \sum_{ss'} \int d^3\boldsymbol{x} \int d^3\boldsymbol{x}' \, \frac{\Psi_s^+(\boldsymbol{x},t)\Psi_{s'}^+(\boldsymbol{x}',t)\Psi_{s'}(\boldsymbol{x}',t)\Psi_s(\boldsymbol{x},t)}{8\pi\epsilon_0|\boldsymbol{x}-\boldsymbol{x}'|}, \quad (21.93)$$

where the summation is over 4-spinor indices. The presentation of the ordering of the field operators was conventionally chosen as the correct ordering in the non-relativistic limit, cf. (18.65), but (21.93) must actually be normal ordered such that the particle and anti-particle creation operators $b_s^+(\boldsymbol{k})$ and $d_s^+(\boldsymbol{k})$ appear leftmost in the Coulomb term in the forms b^+d^+db, d^+d^+dd, etc. Substituting the mode expansions $\Psi \sim b + d^+$ and normal ordering therefore leads to the attractive Coulomb terms between particles and their anti-particles.

The resulting Hamiltonian in Coulomb gauge therefore has the form

$$\begin{aligned} H = \int d^3\boldsymbol{x} \Big(& c\overline{\Psi}(\boldsymbol{x},t)\left[mc - \boldsymbol{\gamma}\cdot(\mathrm{i}\hbar\nabla + q\boldsymbol{A}(\boldsymbol{x},t))\right]\Psi(\boldsymbol{x},t) \\ & + \frac{\epsilon_0}{2}\boldsymbol{E}_\perp^2(\boldsymbol{x},t) + \frac{1}{2\mu_0}\boldsymbol{B}^2(\boldsymbol{x},t)\Big) \\ & + q^2 \sum_{ss'} \int d^3\boldsymbol{x} \int d^3\boldsymbol{x}' \, \frac{\Psi_s^+(\boldsymbol{x},t)\Psi_{s'}^+(\boldsymbol{x}',t)\Psi_{s'}(\boldsymbol{x}',t)\Psi_s(\boldsymbol{x},t)}{8\pi\epsilon_0|\boldsymbol{x}-\boldsymbol{x}'|}. \end{aligned} \quad (21.94)$$

This Hamiltonian yields the corresponding Dirac equation in the Heisenberg form

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\Psi(\boldsymbol{x},t) = [\Psi(\boldsymbol{x},t), H]$$

if canonical anti-commutation relations are used for the spinor field. The Coulomb gauge wave equation (18.10) with the relativistic current density $\boldsymbol{j}$ (21.40) follows in the form

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\boldsymbol{A}(\boldsymbol{x},t) = [\boldsymbol{A}(\boldsymbol{x},t), H], \quad \frac{\partial^2}{\partial t^2}\boldsymbol{A}(\boldsymbol{x},t) = \frac{1}{\hbar^2}[H,[\boldsymbol{A}(\boldsymbol{x},t),H]]. \quad (21.95)$$

if the commutation relations (18.36, 18.39) are used. This confirms the canonical relations between Heisenberg, Schrödinger and Dirac pictures, and the consistency of Coulomb gauge quantization with the transverse δ function (18.27) also in the fully relativistic theory. It also implies appearance of the Dirac picture time evolution operator in the scattering matrix in the now familiar form.

The momentum operator in Coulomb gauge follows from (21.90) and

$$\int d^3\boldsymbol{x}\,\epsilon_0\boldsymbol{E}_\parallel \times \boldsymbol{B} = -\int d^3\boldsymbol{x}\,\epsilon_0\Phi\Delta\boldsymbol{A} = \int d^3\boldsymbol{x}\,\varrho\boldsymbol{A} = q\int d^3\boldsymbol{x}\,\Psi^+\boldsymbol{A}\Psi$$

as

$$\boldsymbol{P} = \int d^3\boldsymbol{x}\left(\Psi^+\frac{\hbar}{\mathrm{i}}\nabla\Psi + \epsilon_0\boldsymbol{E}_\perp \times \boldsymbol{B}\right), \quad (21.96)$$

where boundary terms at infinity were discarded.

21.5 The non-relativistic limit of the Dirac equation

The Dirac basis (21.36) for the γ-matrices is convenient for the non-relativistic limit. Splitting off the time dependence due to the rest mass term

$$\Psi(\boldsymbol{x},t) = \Upsilon(\boldsymbol{x},t)\exp\!\left(-\mathrm{i}\frac{mc^2}{\hbar}t\right) = \begin{pmatrix}\psi(\boldsymbol{x},t)\\ \phi(\boldsymbol{x},t)\end{pmatrix}\exp\!\left(-\mathrm{i}\frac{mc^2}{\hbar}t\right) \tag{21.97}$$

in the Dirac equation (21.38) yields the equations

$$(\mathrm{i}\hbar\partial_t - q\Phi)\psi + c\underline{\boldsymbol{\sigma}}\cdot(\mathrm{i}\hbar\nabla + q\boldsymbol{A})\phi = 0, \tag{21.98}$$

$$(\mathrm{i}\hbar\partial_t - q\Phi + 2mc^2)\phi + c\underline{\boldsymbol{\sigma}}\cdot(\mathrm{i}\hbar\nabla + q\boldsymbol{A})\psi = 0. \tag{21.99}$$

This yields in the non-relativistic regime

$$\phi \simeq -\frac{1}{2mc}\underline{\boldsymbol{\sigma}}\cdot(\mathrm{i}\hbar\nabla + q\boldsymbol{A})\psi \tag{21.100}$$

and substitution into the equation for ψ yields Pauli's equation[7]

$$\mathrm{i}\hbar\partial_t\psi = -\frac{1}{2m}(\hbar\nabla - \mathrm{i}q\boldsymbol{A})^2\psi - \frac{q\hbar}{2m}\underline{\boldsymbol{\sigma}}\cdot\boldsymbol{B}\psi + q\Phi\psi. \tag{21.101}$$

The spin matrices for spin-1/2 Schrödinger fields are the upper block matrices in the spin matrices (21.78) for the full Dirac fields, $\underline{\boldsymbol{S}} = \hbar\underline{\boldsymbol{\sigma}}/2$, see also Section 8.1 and in particular equation (8.12).

If the external magnetic field $\boldsymbol{B}$ is approximately constant over the extension of the wave function $\psi(\boldsymbol{x},t)$ we can use

$$\boldsymbol{A}(\boldsymbol{x},t) = \frac{1}{2}\boldsymbol{B}(t)\times\boldsymbol{x}.$$

Substitution of the vector potential in equation (21.101) then yields the following linear terms in $\boldsymbol{B}$ in the Hamiltonian on the right hand side,

$$\begin{aligned}\mathrm{i}\frac{q\hbar}{2m}(\boldsymbol{B}\times\boldsymbol{x})\cdot\nabla - \frac{q}{m}\boldsymbol{B}\cdot\underline{\boldsymbol{S}} &= -\frac{q}{2m}\boldsymbol{B}\cdot(\boldsymbol{M} + 2\underline{\boldsymbol{S}})\\ &= -\frac{q}{e}\frac{\mu_B}{\hbar}\boldsymbol{B}\cdot(\boldsymbol{M} + 2\underline{\boldsymbol{S}}).\end{aligned} \tag{21.102}$$

[7] W. Pauli, Z. Phys. 43, 601 (1927). Pauli actually only studied the time-independent Schrödinger equation with the Pauli term in the Hamiltonian, and although he mentions Schrödinger in the beginning, he seems to be more comfortable with Heisenberg's matrix mechanics in the paper.

Here $\mu_B = e\hbar/2m$ is the Bohr magneton, and we used the short hand notation $-\mathrm{i}\hbar\boldsymbol{x}\times\nabla \to \boldsymbol{M}$ for the $\boldsymbol{x}$ representation of the angular momentum operator. Recall that this operator is actually given by

$$\boldsymbol{M} = \mathbf{x}\times\mathbf{p} = -\mathrm{i}\hbar\int d^3\boldsymbol{x}\,|\boldsymbol{x}\rangle\boldsymbol{x}\times\nabla\langle\boldsymbol{x}|.$$

Equation (21.102) shows that the Dirac equation explains the double strength magnetic coupling of spin as compared to orbital angular momentum (often denoted as the *magneto-mechanical anomaly of the electron* or the *anomalous magnetic moment of the electron*). The corresponding electromagnetic currents in the non-relativistic regime are

$$\begin{aligned}\varrho &= q\psi^+\psi,\\ \boldsymbol{j} &= cq\left(\psi^+\underline{\boldsymbol{\sigma}}\phi + \phi^+\underline{\boldsymbol{\sigma}}\psi\right)\\ &= -\frac{q}{2m}\left(\psi^+\underline{\boldsymbol{\sigma}}\otimes\underline{\boldsymbol{\sigma}}\cdot(\mathrm{i}\hbar\nabla + q\boldsymbol{A})\psi - (\mathrm{i}\hbar\nabla\psi^+ - q\psi^+\boldsymbol{A})\cdot\underline{\boldsymbol{\sigma}}\otimes\underline{\boldsymbol{\sigma}}\psi\right),\end{aligned}$$

where $\underline{\boldsymbol{\sigma}}\otimes\underline{\boldsymbol{\sigma}}$ is the three-dimensional tensor with the (2×2)-matrix entries $\underline{\sigma}_i\cdot\underline{\sigma}_j$ (we can think of it as a (3×3)-matrix containing (2×2)-matrices as entries). Substitution of

$$\underline{\boldsymbol{\sigma}}\otimes\underline{\boldsymbol{\sigma}} = \underline{1} + \mathrm{i}\boldsymbol{e}_i\otimes\boldsymbol{e}_j\epsilon_{ijk}\underline{\sigma}_k$$

yields

$$\boldsymbol{j} = \frac{q}{2\mathrm{i}m}\left(\psi^+\cdot\hbar\nabla\psi - \hbar\nabla\psi^+\cdot\psi - 2\mathrm{i}q\psi^+\boldsymbol{A}\psi\right) + \boldsymbol{j}_s, \tag{21.103}$$

with a spin term

$$\boldsymbol{j}_s = \frac{q\hbar}{2m}\nabla\times\left(\psi^+\underline{\boldsymbol{\sigma}}\psi\right).$$

However, this term does not accumulate or diminish charges in any volume, $\nabla\cdot\boldsymbol{j}_s = 0$, and can therefore be neglected in the calculation of electric currents.

The non-relativistic approximations for the Lagrange density $\mathcal{L}$, the energy density $\mathcal{H}$ and the momentum density $\mathcal{P}$ are

$$\begin{aligned}\mathcal{L} &= \frac{\mathrm{i}\hbar}{2}\left(\psi^+\cdot\frac{\partial}{\partial t}\psi - \frac{\partial}{\partial t}\psi^+\cdot\psi\right) - q\psi^+\Phi\psi + \frac{q\hbar}{2m}\psi^+\underline{\boldsymbol{\sigma}}\cdot\boldsymbol{B}\psi\\ &\quad + \frac{1}{2m}(\mathrm{i}\hbar\nabla\psi^+ - q\psi^+\boldsymbol{A})\cdot(\mathrm{i}\hbar\nabla\psi + q\boldsymbol{A}\psi) - \frac{1}{4\mu_0}F_{\mu\nu}F^{\mu\nu}, \quad (21.104)\\ \mathcal{H} &= \frac{1}{2m}(\hbar\nabla\psi^+ + \mathrm{i}q\psi^+\boldsymbol{A})\cdot(\hbar\nabla\psi - \mathrm{i}q\boldsymbol{A}\psi) - \frac{q\hbar}{2m}\psi^+\underline{\boldsymbol{\sigma}}\cdot\boldsymbol{B}\psi\\ &\quad + \frac{\epsilon_0}{2}\boldsymbol{E}^2 + \frac{1}{2\mu_0}\boldsymbol{B}^2, \quad (21.105)\end{aligned}$$

$$\mathcal{P} = \frac{\hbar}{2\mathrm{i}}\left(\psi^+\cdot\nabla\psi - \nabla\psi^+\cdot\psi\right) - q\psi^+\boldsymbol{A}\psi + \epsilon_0\boldsymbol{E}\times\boldsymbol{B}. \tag{21.106}$$

The Hamiltonian and momentum operators in Coulomb gauge are

$$\begin{aligned} H = \int d^3\boldsymbol{x}\,\Big(&-\frac{1}{2m}\psi^+(\boldsymbol{x},t)[\hbar\nabla - \mathrm{i}q\boldsymbol{A}(\boldsymbol{x},t)]^2\psi(\boldsymbol{x},t) \\ &+ \frac{\epsilon_0}{2}\boldsymbol{E}_\perp^2(\boldsymbol{x},t) + \frac{1}{2\mu_0}\boldsymbol{B}^2(\boldsymbol{x},t) - \frac{q\hbar}{2m}\psi^+(\boldsymbol{x},t)\underline{\boldsymbol{\sigma}}\cdot\boldsymbol{B}(\boldsymbol{x},t)\psi(\boldsymbol{x},t)\Big) \\ &+ q^2\sum_{ss'=1}^{2}\int d^3\boldsymbol{x}\int d^3\boldsymbol{x}'\,\frac{\psi_s^+(\boldsymbol{x},t)\psi_{s'}^+(\boldsymbol{x}',t)\psi_{s'}(\boldsymbol{x}',t)\psi_s(\boldsymbol{x},t)}{8\pi\epsilon_0|\boldsymbol{x}-\boldsymbol{x}'|}. \end{aligned} \tag{21.107}$$

and (cf. equation (21.96))

$$\boldsymbol{P} = \int d^3\boldsymbol{x}\left(\psi^+\frac{\hbar}{\mathrm{i}}\nabla\psi + \epsilon_0\boldsymbol{E}_\perp\times\boldsymbol{B}\right). \tag{21.108}$$

It is interesting to note that if we write the current density (21.103) as

$$\boldsymbol{j} = \boldsymbol{J} + \frac{q\hbar}{2m}\nabla\times\left(\psi^+\underline{\boldsymbol{\sigma}}\psi\right) = \boldsymbol{J} + \frac{q}{e}\mu_B\nabla\times\left(\psi^+\underline{\boldsymbol{\sigma}}\psi\right)$$

we can write Ampère's law with Maxwell's correction term as

$$\nabla\times\left(\boldsymbol{B} - \frac{q}{e}\mu_0\mu_B\psi^+\underline{\boldsymbol{\sigma}}\psi\right) = \nabla\times\boldsymbol{B}_{class} = \mu_0\boldsymbol{J} + \mu_0\epsilon_0\frac{\partial}{\partial t}\boldsymbol{E},$$

i.e. the "spin density"

$$\boldsymbol{S}(\boldsymbol{x},t) = \frac{\hbar}{2}\psi^+(\boldsymbol{x},t)\underline{\boldsymbol{\sigma}}\psi(\boldsymbol{x},t)$$

adds a spin magnetic field to the magnetic field $\boldsymbol{B}_{class}$ which is generated by orbital currents $\boldsymbol{J}$ and time-dependent electric fields $\boldsymbol{E}$,

$$\boldsymbol{B}(\boldsymbol{x},t) = \boldsymbol{B}_{class}(\boldsymbol{x},t) + \frac{2q}{e\hbar}\mu_0\mu_B\boldsymbol{S}(\boldsymbol{x},t) = \boldsymbol{B}_{class}(\boldsymbol{x},t) + \mu_0\frac{q}{m}\boldsymbol{S}(\boldsymbol{x},t).$$

Higher order terms and spin-orbit coupling

We will discuss higher order terms in the framework of relativistic quantum mechanics, i.e. our basic quantum operators are **x** and **p** etc., but not quantum fields. This also entails a semi-classical approximation for the electromagnetic fields and potentials.

For the discussion of higher order terms, we write the Dirac equation in Schrödinger form,

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

with the Hamilton operator

$$H(t) = (\gamma^0 - 1)mc^2 + q\Phi(\mathbf{x},t) + c\,\boldsymbol{\alpha}\cdot[\mathbf{p} - q\boldsymbol{A}(\mathbf{x},t)]. \tag{21.109}$$

The operator $\boldsymbol{\alpha}$ is

$$\boldsymbol{\alpha} = \gamma^0\boldsymbol{\gamma}, \quad \alpha^i{}_{ab} = \langle a|\alpha^i|b\rangle = \gamma^0{}_{ac}\gamma^i{}_{cb},$$

and $\langle\boldsymbol{x},a|\Upsilon(t)\rangle = \Upsilon_a(\boldsymbol{x},t)$ is the a-th component of the 4-spinor Υ (21.97) in $\boldsymbol{x}$ representation.

We continue to use the Dirac basis (21.36) of γ matrices in this section, such that as a matrix valued vector $\boldsymbol{\alpha}$ is given by

$$\boldsymbol{\alpha} = \begin{pmatrix} \underline{0} & \underline{\boldsymbol{\sigma}} \\ \underline{\boldsymbol{\sigma}} & \underline{0} \end{pmatrix}.$$

The part of the Hamiltonian (21.109) which mixes the upper and lower components of the 4-spinor Υ is

$$K(t) = c\,\boldsymbol{\alpha}\cdot[\mathbf{p} - q\boldsymbol{A}(\mathbf{x},t)].$$

Operators which mix upper and lower 2-spinors in 4-spinors are also denoted as *odd* terms in the Hamiltonian.

We can remove the odd contribution $K(t)$ by using the anti-hermitian operator

$$T(t) = \frac{\gamma^0}{2mc^2}K(t) = \frac{1}{2mc}\boldsymbol{\gamma}\cdot[\mathbf{p} - q\boldsymbol{A}(\mathbf{x},t)],$$

$$[T(t), \gamma^0 mc^2] = -K(t), \tag{21.110}$$

which implies subtraction of $K(t)$ from the new transformed Hamiltonian $\exp[T(t)]H(t)\exp[-T(t)]$. However, we also have to take into account that the transformed state $|\Upsilon_T(t)\rangle = \exp[T(t)]|\Upsilon(t)\rangle$ satisfies the equation

$$\mathrm{i}\hbar\frac{d}{dt}|\Upsilon_T(t)\rangle = \exp[T(t)]H(t)\exp[-T(t)]|\Upsilon(t)\rangle + \mathrm{i}\hbar\frac{d\exp[T(t)]}{dt}\exp[-T(t)]|\Upsilon(t)\rangle.$$

Therefore the transformed Hamiltonian is actually

$$\begin{aligned}
H_T(t) &= \exp[T(t)]H(t)\exp[-T(t)] - \mathrm{i}\hbar\exp[T(t)]\frac{d}{dt}\exp[-T(t)] \\
&= \sum_{n=0}^{\infty}\frac{1}{n!}\overset{n}{[}T(t), H(t)] - \mathrm{i}\hbar\sum_{n=0}^{\infty}\frac{1}{n!}\overset{n}{[}T(t), d/dt] \\
&= \sum_{n=0}^{\infty}\frac{1}{n!}\overset{n}{[}T(t), H(t)] + \mathrm{i}\hbar\sum_{n=1}^{\infty}\frac{1}{n!}\overset{n-1}{[}T(t), dT(t)/dt] \\
&= \sum_{n=0}^{\infty}\frac{1}{n!}\overset{n}{[}T(t), H(t)] - \frac{\mathrm{i}q\hbar}{2mc}\sum_{n=1}^{\infty}\frac{1}{n!}\overset{n-1}{[}T(t), \boldsymbol{\gamma}\cdot\dot{\boldsymbol{A}}(t)].
\end{aligned}$$

We also wish to expand the Hamiltonian up to terms of order $(\mathcal{E}/mc^2)^3$, where $\mathcal{E}$ contains contributions from the kinetic energy of the particle and from its interactions with the electromagnetic fields.

Equation (21.110) implies

$$\begin{aligned}
H_T(t) = {} & (\gamma^0 - 1)mc^2 + q\Phi(t) + mc^2\sum_{n=2}^{4}\frac{1}{n!}\overset{n}{[}T(t), \gamma^0] \\
& + \sum_{n=1}^{3}\frac{1}{n!}\overset{n}{[}T(t), q\Phi(t) + K(t)] - \frac{\mathrm{i}q\hbar}{2mc}\boldsymbol{\gamma}\cdot\dot{\boldsymbol{A}}(t) \\
& - \frac{\mathrm{i}q\hbar}{2mc}\sum_{n=1}^{2}\frac{1}{(n+1)!}\overset{n}{[}T(t), \boldsymbol{\gamma}\cdot\dot{\boldsymbol{A}}(t)] + \mathcal{O}\left(\frac{\mathcal{E}}{mc^2}\right)^4.
\end{aligned}$$

The relevant commutators are

$$[T(t), q\Phi(t)] - \frac{\mathrm{i}q\hbar}{2mc}\boldsymbol{\gamma}\cdot\dot{\boldsymbol{A}}(t) = \frac{\mathrm{i}q\hbar}{2mc}\boldsymbol{\gamma}\cdot\boldsymbol{E}(\mathbf{x}, t),$$

$$\begin{aligned}
& \overset{2}{[}T(t), q\Phi(t)] - \frac{\mathrm{i}q\hbar}{2mc}[T(t), \boldsymbol{\gamma}\cdot\dot{\boldsymbol{A}}(t)] = \frac{\mathrm{i}q\hbar}{2mc}[T(t), \boldsymbol{\gamma}\cdot\boldsymbol{E}(t)] \\
& = -\frac{q\hbar^2}{4m^2c^2}\nabla\cdot\boldsymbol{E}(\mathbf{x}, t) - \mathrm{i}\frac{q\hbar^2}{4m^2c^2}\big(\nabla\times\boldsymbol{E}(\mathbf{x}, t)\big)\cdot\begin{pmatrix}\underline{\boldsymbol{\sigma}} & \underline{0} \\ \underline{0} & \underline{\boldsymbol{\sigma}}\end{pmatrix} \\
& \quad - \frac{q\hbar}{2m^2c^2}\big(\boldsymbol{E}(\mathbf{x}, t)\times[\mathbf{p} - q\boldsymbol{A}(\mathbf{x}, t)]\big)\cdot\begin{pmatrix}\underline{\boldsymbol{\sigma}} & \underline{0} \\ \underline{0} & \underline{\boldsymbol{\sigma}}\end{pmatrix},
\end{aligned}$$

$$[T(t), K(t)] = \frac{\gamma^0}{mc^2}K^2(t) = \frac{\gamma^0}{m}[\mathbf{p} - q\boldsymbol{A}(\mathbf{x}, t)]^2 - \frac{q\hbar}{m}\boldsymbol{B}(\mathbf{x}, t)\cdot\begin{pmatrix}\underline{\boldsymbol{\sigma}} & \underline{0} \\ \underline{0} & -\underline{\boldsymbol{\sigma}}\end{pmatrix},$$

$$\overset{2}{[}T(t),K(t)] = -\frac{1}{m^2c^4}K^3(t), \quad \overset{3}{[}T(t),K(t)] = -\frac{\gamma^0}{m^3c^6}K^4(t).$$

and

$$mc^2\,\overset{2}{[}T(t),\gamma^0] = [K(t),T(t)] = -\frac{\gamma^0}{mc^2}K^2(t),$$
$$mc^2\,\overset{3}{[}T(t),\gamma^0] = \frac{1}{m^2c^4}K^3(t), \quad mc^2\,\overset{4}{[}T(t),\gamma^0] = \frac{\gamma^0}{m^3c^6}K^4(t).$$

We don't need to evaluate the final higher order commutator

$$C^{(3)}_{odd}(t) = \overset{3}{[}T(t),q\Phi(t)] - \frac{\mathrm{i}q\hbar}{2mc}\,\overset{2}{[}T(t),\boldsymbol{\gamma}\cdot\dot{\boldsymbol{A}}(t)],$$

because this is an odd term of order $(\mathcal{E}/mc^2)^3$, which is eliminated in the next step through a unitary transformation, to which it contributes in order $(\mathcal{E}/mc^2)^4$. We only need to observe that $C^{(3)}_{odd}(t)$ contains one term proportional to $\boldsymbol{\gamma}$, and other terms proportional to

$$\gamma^i\cdot\begin{pmatrix}\underline{\sigma}^j & \underline{0}\\ \underline{0} & \underline{\sigma}^j\end{pmatrix} = \delta^{ij}\begin{pmatrix}\underline{0} & \underline{1}\\ -\underline{1} & \underline{0}\end{pmatrix} + \mathrm{i}\epsilon^{ijk}\gamma_k,$$

such that $\{\gamma^0, C^{(3)}_{odd}(t)\} = 0$. This will become relevant for the elimination of $C^{(3)}_{odd}(t)$ in the next step.

However, for now our transformed Hamiltonian is

$$\begin{aligned}H_T(t) = {} & (\gamma^0-1)mc^2 + q\Phi(t) + \frac{\gamma^0}{2mc^2}K^2(t) - \frac{\gamma^0}{8m^3c^6}K^4(t)\\ & - \frac{q\hbar^2}{8m^2c^2}\nabla\cdot\boldsymbol{E}(t) - \mathrm{i}\frac{q\hbar^2}{8m^2c^2}\big(\nabla\times\boldsymbol{E}(t)\big)\cdot\begin{pmatrix}\underline{\boldsymbol{\sigma}} & \underline{0}\\ \underline{0} & \underline{\boldsymbol{\sigma}}\end{pmatrix}\\ & - \frac{q\hbar}{4m^2c^2}\big(\boldsymbol{E}(t)\times[\mathbf{p}-q\boldsymbol{A}(\mathbf{x},t)]\big)\cdot\begin{pmatrix}\underline{\boldsymbol{\sigma}} & \underline{0}\\ \underline{0} & \underline{\boldsymbol{\sigma}}\end{pmatrix}\\ & + \frac{\mathrm{i}q\hbar}{2mc}\boldsymbol{\gamma}\cdot\boldsymbol{E}(t) - \frac{1}{3m^2c^4}K^3(t) + \frac{1}{6}C^{(3)}_{odd}(t) + \mathcal{O}\left(\frac{\mathcal{E}}{mc^2}\right)^4.\end{aligned}$$

The last line contains three odd contributions

$$L(t) = \frac{\mathrm{i}q\hbar}{2mc}\boldsymbol{\gamma}\cdot\boldsymbol{E}(t) - \frac{1}{3m^2c^4}K^3(t) + \frac{1}{6}C^{(3)}_{odd}(t),$$

which we can eliminate exactly as in the previous step by using a unitary transformation $|\Upsilon_{WT}(t)\rangle = \exp[W(t)]|\Upsilon_T(t)\rangle$ with

$$W(t) = \frac{\gamma^0}{2mc^2}L(t) = \frac{\mathrm{i}q\hbar}{4m^2c^3}\boldsymbol{\alpha}\cdot\boldsymbol{E}(t) - \frac{\gamma^0}{6m^3c^6}K^3(t) + \mathcal{O}\left(\frac{\mathcal{E}}{mc^2}\right)^4.$$

This yields a new Hamiltonian

$$\begin{aligned} H_{WT}(t) &= \exp[W(t)]H_T(t)\exp[-W(t)] - \mathrm{i}\hbar\exp[W(t)]\frac{d}{dt}\exp[-W(t)] \\ &= \sum_{n=0}^{\infty}\frac{1}{n!}\overset{n}{[}W(t), H_T(t)] + \mathrm{i}\hbar\sum_{n=1}^{\infty}\frac{1}{n!}\overset{n-1}{[}W(t), dW(t)/dt], \end{aligned}$$

which is in the required order

$$\begin{aligned} H_{WT}(t) = {} & (\gamma^0 - 1)mc^2 + q\Phi(t) + \frac{\gamma^0}{2mc^2}K^2(t) - \frac{\gamma^0}{8m^3c^6}K^4(t) \\ & - \frac{q\hbar^2}{8m^2c^2}\nabla\cdot\boldsymbol{E}(t) - \mathrm{i}\frac{q\hbar^2}{8m^2c^2}\big(\nabla\times\boldsymbol{E}(t)\big)\cdot\begin{pmatrix}\underline{\boldsymbol{\sigma}} & \underline{0} \\ \underline{0} & \underline{\boldsymbol{\sigma}}\end{pmatrix} \\ & - \frac{q\hbar}{4m^2c^2}\big(\boldsymbol{E}(t)\times[\mathbf{p} - q\boldsymbol{A}(\mathbf{x},t)]\big)\cdot\begin{pmatrix}\underline{\boldsymbol{\sigma}} & \underline{0} \\ \underline{0} & \underline{\boldsymbol{\sigma}}\end{pmatrix} \\ & - \frac{q\gamma^0}{6m^3c^6}[K^3(t), \Phi(t)] + \frac{\mathrm{i}q\hbar}{8m^3c^5}[\boldsymbol{\alpha}\cdot\boldsymbol{E}(t), \gamma^0K^2(t)] \\ & + \mathrm{i}\hbar\frac{dW(t)}{dt} + \mathcal{O}\left(\frac{\mathcal{E}}{mc^2}\right)^4. \end{aligned}$$

This contains again an odd piece

$$M(t) = \mathrm{i}\hbar\frac{dW(t)}{dt} - \frac{q\gamma^0}{6m^3c^6}[K^3(t), \Phi(t)] + \frac{\mathrm{i}q\hbar}{8m^3c^5}[\boldsymbol{\alpha}\cdot\boldsymbol{E}(t), \gamma^0K^2(t)]$$

which is eliminated by another unitary transformation of the form $|\Upsilon_{FWT}(t)\rangle = \exp[F(t)]|\Upsilon_{WT}(t)\rangle$ with

$$F(t) = \frac{\gamma^0}{2mc^2}M(t) = -\frac{q\hbar^2}{8m^3c^5}\boldsymbol{\gamma}\cdot\dot{\boldsymbol{E}}(t) + \mathcal{O}\left(\frac{\mathcal{E}}{mc^2}\right)^4.$$

The resulting Hamiltonian after this transformation still contains an odd piece

$$N(t) = -\mathrm{i}\frac{q\hbar^3}{8m^3c^5}\boldsymbol{\gamma}\cdot\ddot{\boldsymbol{E}}(t)$$

which is eliminated in a final transformation

$$G(t) = \frac{\gamma^0}{2mc^2}N(t) = \mathcal{O}\left(\frac{\mathcal{E}}{mc^2}\right)^4.$$

Therefore up to terms of order $\mathcal{O}(\mathcal{E}/mc^2)^4$, we finally find an equation which is diagonal in upper and lower 2-spinors

$$|\Upsilon_{FWT}(t)\rangle = \exp[F(t)]\exp[W(t)]\exp[T(t)]|\Upsilon(t)\rangle, \quad (21.111)$$

$$\mathrm{i}\hbar\frac{d}{dt}|\Upsilon_{FWT}(t)\rangle = H_{FWT}(t)|\Upsilon_{FWT}(t)\rangle \quad (21.112)$$

with

$$\begin{aligned} H_{FWT}(t) = {} & (\gamma^0 - 1)mc^2 + q\Phi(t) + \frac{\gamma^0}{2mc^2}K^2(t) - \frac{\gamma^0}{8m^3c^6}K^4(t) \\ & - \frac{q\hbar^2}{8m^2c^2}\nabla\cdot\boldsymbol{E}(t) - \mathrm{i}\frac{q\hbar^2}{8m^2c^2}\big(\nabla\times\boldsymbol{E}(t)\big)\cdot\begin{pmatrix}\underline{\boldsymbol{\sigma}} & \underline{0}\\ \underline{0} & \underline{\boldsymbol{\sigma}}\end{pmatrix} \\ & - \frac{q\hbar}{4m^2c^2}\big(\boldsymbol{E}(t)\times[\mathbf{p} - q\boldsymbol{A}(\mathbf{x},t)]\big)\cdot\begin{pmatrix}\underline{\boldsymbol{\sigma}} & \underline{0}\\ \underline{0} & \underline{\boldsymbol{\sigma}}\end{pmatrix}. \end{aligned} \quad (21.113)$$

The transformation (21.111, 21.113) is known as a Foldy-Wouthuysen transformation[8].

The Hamiltonian acting on the upper 2-spinor is

$$\begin{aligned} H(t) = {} & \frac{[\mathbf{p} - q\boldsymbol{A}(\mathbf{x},t)]^2}{2m} + q\Phi(\mathbf{x},t) - \frac{q\hbar}{2m}\boldsymbol{B}(\mathbf{x},t)\cdot\underline{\boldsymbol{\sigma}} - \frac{q\hbar^2}{8m^2c^2}\nabla\cdot\boldsymbol{E}(\mathbf{x},t) \\ & - \frac{q\hbar}{8m^2c^2}\big(\mathrm{i}\hbar\nabla\times\boldsymbol{E}(\mathbf{x},t) + 2\boldsymbol{E}(\mathbf{x},t)\times[\mathbf{p} - q\boldsymbol{A}(\mathbf{x},t)]\big)\cdot\underline{\boldsymbol{\sigma}} \\ & - \frac{1}{8m^3c^2}\left([\mathbf{p} - q\boldsymbol{A}(\mathbf{x},t)]^2 - q\hbar\boldsymbol{B}(\mathbf{x},t)\cdot\underline{\boldsymbol{\sigma}}\right)^2. \end{aligned} \quad (21.114)$$

The first three terms are again the Pauli Hamiltonian from (21.101).

It is of interest to write some of the higher order terms in the Hamiltonian (21.114) also in terms of the charge density $\varrho(\boldsymbol{x},t)$ which generates the electromagnetic fields.

The term

$$-\frac{q\hbar^2}{8m^2c^2}\nabla\cdot\boldsymbol{E}(\mathbf{x},t) = -\frac{q\hbar^2}{8m^2c^2\epsilon_0}\varrho(\mathbf{x},t) \quad (21.115)$$

[8] L.L. Foldy, S.A. Wouthuysen, Phys. Rev. 78, 29 (1950).

amounts to a contact interaction between the particles described by equation (21.112) (e.g. electrons) and the particles which generate the electromagnetic fields. This term is known as the Darwin term. The contact interaction has the counter-intuitive property to lower the interaction energy between like charges, but recall that it emerged from eliminating the anti-particle components up to terms of order $\mathcal{O}(\mathcal{E}/mc^2)^4$. It should not surprise us that a positronic component in electron wave functions contributes an attractive term to the electron-electron interaction. The Hamiltonian (21.114) is in excellent agreement with spectroscopy if radiative corrections are also taken into account, see e.g. [18].

The term

$$- \mathrm{i}\frac{q\hbar^2}{8m^2c^2}\big(\nabla \times \boldsymbol{E}(\mathbf{x},t)\big)\cdot \underline{\boldsymbol{\sigma}} = \mathrm{i}\frac{q\hbar}{4m^2c^2}\dot{\boldsymbol{B}}(\mathbf{x},t)\cdot \underline{\boldsymbol{S}} \tag{21.116}$$

is apparently a coupling between spin $\underline{\boldsymbol{S}} = \hbar\underline{\boldsymbol{\sigma}}/2$ and induced potentials from time-dependent charge-current distributions.

In the static case we can write the $\boldsymbol{E}(\mathbf{x}) \times \mathbf{p}$ term in (21.114) in the form

$$- \frac{q}{2m^2c^2}\big(\boldsymbol{E}(\mathbf{x}) \times \mathbf{p}\big)\cdot \underline{\boldsymbol{S}} = - \frac{\mu_0 q}{8\pi m^2}\int d^3\boldsymbol{x}'\, \frac{\varrho(\boldsymbol{x}')}{|\mathbf{x}-\boldsymbol{x}'|^3}\boldsymbol{M}(\mathbf{x}-\boldsymbol{x}',\mathbf{p})\cdot \underline{\boldsymbol{S}}.$$

Here

$$\boldsymbol{M}(\mathbf{x}-\boldsymbol{x}',\mathbf{p}) = (\mathbf{x}-\boldsymbol{x}')\times \mathbf{p}$$

is the orbital angular momentum operator with respect to the point $\boldsymbol{x}'$, and the $\boldsymbol{E}(\mathbf{x}) \times \mathbf{p}$ term apparently contains a charge weighted sum over angular momentum operators. The $\boldsymbol{E}(\mathbf{x}) \times \mathbf{p}$ term is therefore the origin of spin-orbit coupling. In particular, for a radially symmetric charge distribution

$$\boldsymbol{E}(\boldsymbol{x}) = -\frac{\boldsymbol{x}}{r}\frac{d\Phi(r)}{dr}$$

one finds

$$- \frac{q}{2m^2c^2}\big(\boldsymbol{E}(\mathbf{x}) \times \mathbf{p}\big)\cdot \underline{\boldsymbol{S}} = \frac{q}{2m^2c^2 r}\frac{d\Phi(r)}{dr}\boldsymbol{M}\cdot \underline{\boldsymbol{S}}. \tag{21.117}$$

This implies equation (8.20) for spin-orbit coupling in hydrogen atoms.

So far we have emphasized the emergence of $\boldsymbol{M}\cdot\boldsymbol{S}$ terms from the $\boldsymbol{E}(\mathbf{x})\times\mathbf{p}$ term, and historically the coupling of spin and orbital angular momentum had provided the initial motivation for the designation as spin-orbit coupling term. However, the direct coupling of orbital momentum $\boldsymbol{p}$ and spin provides just as good a reason for the name spin-orbit coupling, and another important special case of the $\boldsymbol{E}(\mathbf{x}) \times \mathbf{p}$ term arises for a uni-directional electric field e.g. in z direction. In this case the term takes the form

$$- \frac{q}{2m^2c^2}\big(\boldsymbol{E}(\mathbf{x}) \times \mathbf{p}\big)\cdot \boldsymbol{S} = - \frac{q}{2m^2c^2}E_z(\mathrm{z})\left(\mathrm{p}_x S_y - \mathrm{p}_y S_x\right). \tag{21.118}$$

For homogeneous electric field this yields a spin-orbit coupling term of the form $\alpha_R(\mathrm{p}_x S_y - \mathrm{p}_y S_x)$ with constant α_R. This particular form of a spin-orbit coupling term is known as a Rashba term[9]. Spin-orbit coupling was always relevant not only for atomic and molecular spectroscopy, but also for electronic energy band structure in materials where they are often significantly enhanced e.g. due to low effective masses. In recent years spin-orbit coupling terms in low-dimensional systems, and Rashba terms in particular, have also attracted a lot of interest because of their relevance for spintronics[10].

21.6 Covariant quantization of the Maxwell field

We have seen in Section 18.2 how to quantize the Maxwell field and describe photons in Coulomb gauge. This is useful if our problem contains non-relativistic charged particles, since the Hamiltonian in Coulomb gauge conveniently describes the electromagnetic interaction between the charged particles through Coulomb terms. The free interaction picture photon operators $\boldsymbol{A}(\boldsymbol{x},t)$ or the corresponding Schrödinger picture operators $\boldsymbol{A}(\boldsymbol{x})$ are then only needed for the calculation of absorption, emission or scattering of external photons. Exchange of virtual photons provides only small corrections to Coulomb interactions for non-relativistic charged particles. The relevant Hamiltonian is (21.107) with Schrödinger fields and Coulomb terms for all the different kinds of charged particles.

Coulomb gauge can also be used for problems involving relativistic fermions. These can be described by the Hamiltonian (21.94) including Dirac fields and Coulomb interaction terms for all the different kinds of spin-$1/2$ particles in the problem. Indeed, we will calculate basic scattering processes involving relativistic charged particles in Sections 22.2 and 22.4 in Coulomb gauge, and the calculations will explicitly show how the Coulomb interaction terms between charged particles dominate over photon exchange terms if the kinetic energies of the charged particles are small compared to their rest energies, see in particular equation (22.29).

However, if the problem indeed contains relativistic charged particles, then the interaction of those particles with other charged particles is more conveniently described through a covariant quantization of photons in Lorentz gauge,

$$\partial_\mu A^\mu(x) = 0. \tag{21.119}$$

[9]E.I. Rashba, Sov. Phys. Solid State 2, 1109 (1960); Yu.A. Bychkov, E.I. Rashba, JETP Lett. 39, 78 (1984); J. Phys. C 17, 6039 (1984).

[10]See e.g. J. Nitta, T. Akazaki, H. Takayanagi, T. Enoki, Phys. Rev. Lett. 78, 1335 (1997); D. Grundler, Phys. Rev. Lett. 84, 6074 (2000); J. Sinova *et al.*, Phys. Rev. Lett. 92, 126603 (2004); E.Y. Sherman, D.J. Lockwood, Phys. Rev. B 72, 125340 (2005); K.C. Hall *et al.*, Appl. Phys. Lett. 86, 202114 (2005); P. Pietiläinen, T. Chakraborty, Phys. Rev. B 73, 155315 (2006); E. Cappelluti, C. Grimaldi, F. Marsiglio, Phys. Rev. Lett. 98, 167002 (2007).

Suppose the potential $\mathcal{A}_\mu(x)$ does not satisfy the Lorentz gauge condition. We can construct the Lorentz gauge vector potential $A^\mu(x)$ by performing a gauge transformation

$$A_\mu(x) = \mathcal{A}_\mu(x) + \partial_\mu f(x) \tag{21.120}$$

with

$$\begin{aligned} f(x) &= \int d^4x'\, G_d^{(m=0)}(x-x')\partial'_\mu \mathcal{A}^\mu(x') \\ &= \int d^3\boldsymbol{x}' \frac{1}{4\pi|\boldsymbol{x}-\boldsymbol{x}'|}\partial'_\mu \mathcal{A}^\mu(x')\Big|_{ct'=ct-|\boldsymbol{x}-\boldsymbol{x}'|}. \end{aligned} \tag{21.121}$$

Here

$$G_d^{(m=0)}(x) = \frac{1}{c}G_d^{(r,m=0)}(\boldsymbol{x},t) = \frac{1}{4\pi r}\delta(r-ct)$$

is the retarded massless scalar Green's function, cf. (J.37, J.60). This also helps us to solve Maxwell's equations in Lorentz gauge,

$$\partial_\mu \partial^\mu A^\nu(x) = -\mu_0 j^\nu(x) \tag{21.122}$$

in the form

$$A^\mu(x) = A^\mu_{LW}(x) + A^\mu_D(x), \tag{21.123}$$

where the Liénard-Wiechert potentials

$$\begin{aligned} A^\mu_{LW}(x) &= \mu_0 \int d^4x'\, G_d^{(m=0)}(x-x')j^\mu(x') \\ &= \frac{\mu_0}{4\pi}\int d^3\boldsymbol{x}'\, \frac{1}{|\boldsymbol{x}-\boldsymbol{x}'|}j^\mu\big(\boldsymbol{x}', ct - |\boldsymbol{x}-\boldsymbol{x}'|\big) \end{aligned} \tag{21.124}$$

solve the inhomogeneous Maxwell equations (21.122) and satisfy the Lorentz gauge condition due to charge conservation. The remainder $A^\mu_D(x)$ must therefore satisfy

$$\partial_\mu \partial^\mu A^\nu_D(x) = 0, \quad \partial_\mu A^\mu_D(x) = 0. \tag{21.125}$$

To quantize this, we observe that Maxwell's equations in Lorentz gauge follow from the Lagrange density of electromagnetic fields (18.1) if we take into account the Lorentz gauge condition,

$$\mathcal{L} = A_\mu j^\mu - \frac{1}{2\mu_0}\partial_\nu A_\mu \cdot \partial^\nu A^\mu. \tag{21.126}$$

This yields canonically conjugate momentum fields for all components of the vector potential,

$$\Pi_\mu = \frac{\partial\mathcal{L}}{\partial\dot{A}^\mu} = \epsilon_0\dot{A}_\mu.$$

The principles of canonical quantization and the Lorentz gauge condition then motivate the following quantization condition for electromagnetic potentials in Lorentz gauge (with $k^0 = |\boldsymbol{k}|$),

$$[A_\mu(x), \dot{A}_\nu(x')]_{t=t'} = \frac{\mathrm{i}\hbar}{\epsilon_0}\int d^3\boldsymbol{k}\left(\eta_{\mu\nu} - \frac{k_\mu k_\nu}{k^2 - \mathrm{i}\epsilon}\right)\frac{\exp[\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{x}-\boldsymbol{x}')]}{(2\pi)^3}.$$

The general solution of (21.125)

$$A_D^\mu(x) = \langle x, \mu|A_D\rangle = \sqrt{\frac{\hbar\mu_0 c}{(2\pi)^3}}$$
$$\times\int\frac{d^3\boldsymbol{k}}{\sqrt{2|\boldsymbol{k}|}}\sum_{\alpha=1}^{3}\epsilon_\alpha^\mu(\boldsymbol{k})\Big(a_\alpha(\boldsymbol{k})\exp(\mathrm{i}k\cdot x) + a_\alpha^+(\boldsymbol{k})\exp(-\mathrm{i}k\cdot x)\Big), \quad (21.127)$$

$$k\cdot\epsilon_\alpha(\boldsymbol{k}) = 0, \quad \sum_{\alpha=1}^{3}\epsilon_\alpha^\mu(\boldsymbol{k})\epsilon_\alpha^\nu(\boldsymbol{k}) = \eta^{\mu\nu} - \frac{k^\mu k^\nu}{k^2 - \mathrm{i}\epsilon},$$

satisfies the quantization condition if

$$[a_\alpha(\boldsymbol{k}), a_\beta^+(\boldsymbol{k}')] = \delta_{\alpha\beta}\delta(\boldsymbol{k}-\boldsymbol{k}') \quad (21.128)$$

and the other commutators vanish.

A possible choice for the polarization vectors $\epsilon_\alpha^\mu(\boldsymbol{k})$ is e.g. to choose $\epsilon_1^\mu(\boldsymbol{k})$ and $\epsilon_2^\mu(\boldsymbol{k})$ as spatial orthonormal vectors without time-like components and perpendicular to $\boldsymbol{k}$ such that

$$\sum_{\alpha=1}^{2}\boldsymbol{\epsilon}_\alpha(\boldsymbol{k})\otimes\boldsymbol{\epsilon}_\alpha(\boldsymbol{k}) = \underline{1} - \hat{\boldsymbol{k}}\otimes\hat{\boldsymbol{k}},$$

and choose

$$\epsilon_3(\boldsymbol{k}) = \frac{(|\boldsymbol{k}|, k^0\hat{\boldsymbol{k}})}{\sqrt{-k^2 + \mathrm{i}\epsilon}}.$$

This formalism can be motivated as a limiting case of the quantization of massive vector fields, and it has the advantage of faster and easier calculation of scattering amplitudes involving electromagnetic interactions of relativistic charged particles, because there are no separate amplitudes for photon exchange and Coulomb interactions, which need to be added to give the full scattering amplitude. The spatially longitudinal photons generated by $a_3^+(\boldsymbol{k})$, $\boldsymbol{k}\cdot\boldsymbol{\epsilon}_3(\boldsymbol{k}) = k^0\epsilon_3^0(\boldsymbol{k}) \neq 0$, incorporate the contributions from the Coulomb interactions[11]. Why then don't we see photon states $a_3^+(\boldsymbol{k})|0\rangle$? These photon states are actually spurious gauge degrees of freedom. We could perform another gauge transformation

$$A_\mu(x) \to \tilde{A}_\mu(x) = A_\mu(x) + \partial_\mu g(x) \tag{21.129}$$

with

$$g(\boldsymbol{x},t) = \int_{-\infty}^{t} dt' \left(cA^0(\boldsymbol{x},t') - \int d^3\boldsymbol{x}' \, \frac{\varrho(\boldsymbol{x}',t')}{4\pi\epsilon_0|\boldsymbol{x}-\boldsymbol{x}'|} \right) + \int d^3\boldsymbol{x}' \, \frac{\nabla'\cdot\boldsymbol{A}(\boldsymbol{x}',-\infty)}{4\pi|\boldsymbol{x}-\boldsymbol{x}'|} = \int d^3\boldsymbol{x}' \, \frac{\nabla'\cdot\boldsymbol{A}(\boldsymbol{x}',t)}{4\pi|\boldsymbol{x}-\boldsymbol{x}'|}, \tag{21.130}$$

which takes us right back to Coulomb gauge,

$$\tilde{A}^0(x) = \int d^3\boldsymbol{x}' \, \frac{\varrho(\boldsymbol{x}',t)c}{4\pi\epsilon_0|\boldsymbol{x}-\boldsymbol{x}'|}, \quad \nabla\cdot\tilde{\boldsymbol{A}}(x) = 0,$$

without any freely oscillating time-like component. Since $a_3^+(\boldsymbol{k})|0\rangle$ was the only photon state with a time-like component, (21.129) has removed that photon state. We can think of the photons with longitudinal spatial components and corresponding time-like components as virtual place holders for the Coulomb interaction.

21.7 Problems

21.1. Show that for an appropriate class of integration contours $\mathcal{C}$ in the complex k^0 plane the scalar propagator (21.9) can be written in the form

$$\mathcal{K}(x) = -\frac{1}{(2\pi)^4 c} \oint_{\mathcal{C}} dk^0 \int d^3\boldsymbol{k} \, \frac{\exp(\mathrm{i}k\cdot x)}{k^2 + (mc/\hbar)^2}.$$

[11] Of course, this implies that one cannot naively invoke Hamiltonians with Coulomb interaction terms if we describe photons in Lorentz gauge. Otherwise we would overcount interactions. Remember that the Coulomb interaction terms came from the contributions to Hamiltonians from electromagnetic fields *in Coulomb gauge*, see Section 21.4.

21.2. We have discussed the non-relativistic limit of the Klein-Gordon field in the case $|\langle b^+(\boldsymbol{k})\rangle| \ll |\langle a(\boldsymbol{k})\rangle|$. However, there must also exist a non-relativistic limit for the anti-particles. How does the non-relativistic limit work in the case of negligible particle amplitude $|\langle a(\boldsymbol{k})\rangle| \ll |\langle b^+(\boldsymbol{k})\rangle|$?

21.3. Derive the energy density $\mathcal{H}$ and the momentum density $\mathcal{P}$ for the real Klein-Gordon field.

21.4. Calculate the non-relativistic limits for the Hamilton operator H and the momentum operator $\boldsymbol{P}$ of the real Klein-Gordon field.

21.5. Derive the energy-momentum tensor for QED with scalar matter (21.2),

$$\begin{aligned} T_\nu{}^\mu =& -\eta_\nu{}^\mu \hbar c^2 \left(\partial_\rho \phi^+ + \mathrm{i}\frac{q}{\hbar}\phi^+ A_\rho\right)\left(\partial^\rho \phi - \mathrm{i}\frac{q}{\hbar}A^\rho \phi\right) - \eta_\nu{}^\mu \frac{m^2c^4}{\hbar}\phi^+\phi \\ & -\eta_\nu{}^\mu \frac{1}{4\mu_0}F_{\rho\sigma}F^{\rho\sigma} + \hbar c^2\left(\partial_\nu \phi^+ + \mathrm{i}\frac{q}{\hbar}\phi^+ A_\nu\right)\left(\partial^\mu \phi - \mathrm{i}\frac{q}{\hbar}A^\mu \phi\right) \\ & + \hbar c^2 \left(\partial^\mu \phi^+ + \mathrm{i}\frac{q}{\hbar}\phi^+ A^\mu\right)\left(\partial_\nu \phi - \mathrm{i}\frac{q}{\hbar}A_\nu \phi\right) + \frac{1}{\mu_0}F_{\nu\rho}F^{\mu\rho}. \end{aligned} \tag{21.131}$$

The corresponding densities of energy, momentum, and energy current are

$$\begin{aligned} \mathcal{H} = T^{00} =& \frac{\epsilon_0}{2}\boldsymbol{E}^2 + \frac{1}{2\mu_0}\boldsymbol{B}^2 + \frac{m^2c^4}{\hbar}\phi^+\phi + \hbar\left(\dot{\phi}^+ - \mathrm{i}\frac{q}{\hbar}\phi^+\Phi\right)\left(\dot{\phi} + \mathrm{i}\frac{q}{\hbar}\Phi\phi\right) \\ & + \hbar c^2 \left(\nabla\phi^+ + \mathrm{i}\frac{q}{\hbar}\phi^+\boldsymbol{A}\right)\cdot\left(\nabla\phi - \mathrm{i}\frac{q}{\hbar}\boldsymbol{A}\phi\right), \end{aligned} \tag{21.132}$$

$$\begin{aligned} \mathcal{P} = \frac{1}{c}\boldsymbol{e}_i T^{i0} =& \epsilon_0 \boldsymbol{E}\times\boldsymbol{B} - \hbar\left(\dot{\phi}^+ - \mathrm{i}\frac{q}{\hbar}\phi^+\Phi\right)\left(\nabla\phi - \mathrm{i}\frac{q}{\hbar}\boldsymbol{A}\phi\right) \\ & - \hbar\left(\nabla\phi^+ + \mathrm{i}\frac{q}{\hbar}\phi^+\boldsymbol{A}\right)\left(\dot{\phi} + \mathrm{i}\frac{q}{\hbar}\Phi\phi\right), \end{aligned} \tag{21.133}$$

$$\mathcal{S} = c\boldsymbol{e}_i T^{0i} = c^2\mathcal{P}.$$

Solution. The Lagrange density for quantum electrodynamics with scalar matter is

$$\mathcal{L} = -\hbar c^2 \left(\partial\phi^+ + \mathrm{i}\frac{q}{\hbar}\phi^+ A\right)\cdot\left(\partial\phi - \mathrm{i}\frac{q}{\hbar}A\phi\right) - \frac{m^2c^4}{\hbar}\phi^+\cdot\phi - \frac{1}{4\mu_0}F_{\mu\nu}F^{\mu\nu}.$$

This yields according to (16.16) a conserved energy-momentum tensor

$$\Theta_\mu{}^\nu = \eta_\mu{}^\nu \mathcal{L} - \partial_\mu\phi^+ \frac{\partial\mathcal{L}}{\partial(\partial_\nu\phi^+)} - \partial_\mu\phi\frac{\partial\mathcal{L}}{\partial(\partial_\nu\phi)} - \partial_\mu A_\lambda \frac{\partial\mathcal{L}}{\partial(\partial_\nu A_\lambda)}$$

$$= \eta_\mu{}^\nu \mathcal{L} + \hbar c^2 \partial_\mu \phi^+ \left(\partial^\nu \phi - \mathrm{i}\frac{q}{\hbar} A^\nu \phi \right) + \hbar c^2 \left(\partial^\nu \phi^+ + \mathrm{i}\frac{q}{\hbar} \phi^+ A^\nu \right) \partial_\mu \phi$$
$$+ \frac{1}{\mu_0} \partial_\mu A_\lambda F^{\nu\lambda}.$$

To find a gauge invariant energy-momentum tensor we add the identically conserved improvement term

$$-\frac{1}{\mu_0}\partial_\lambda \left(A_\mu F^{\nu\lambda}\right) = -\frac{1}{\mu_0}\partial_\lambda A_\mu F^{\nu\lambda} - \frac{1}{\mu_0} A_\mu \partial_\lambda F^{\nu\lambda}$$
$$= -\frac{1}{\mu_0}\partial_\lambda A_\mu F^{\nu\lambda} + \mathrm{i}qc^2 \left(\phi^+ A_\mu \cdot \partial^\nu \phi - \partial^\nu \phi^+ \cdot A_\mu \phi\right) + 2\frac{q^2 c^2}{\hbar} \phi^+ A_\mu A^\nu \phi,$$

where Maxwell's equations

$$\partial_\mu F^{\mu\nu} = -\mu_0 \frac{\partial \mathcal{L}}{\partial A_\nu} = \mathrm{i}\frac{q}{\epsilon_0}\left(\phi^+ \cdot \partial^\nu \phi - \partial^\nu \phi^+ \cdot \phi\right) + 2\frac{q^2}{\epsilon_0 \hbar} \phi^+ A^\nu \phi$$

were used. This yields the gauge invariant tensor (21.131) from

$$T_\mu{}^\nu = \Theta_\mu{}^\nu - \frac{1}{\mu_0}\partial_\lambda \left(A_\mu F^{\nu\lambda}\right).$$

21.6. If we write the solution (21.5) of the free Klein-Gordon equation as the sum of the positive and negative energy components,

$$\phi(x) = \phi_+(x) + \phi_-(x),$$
$$\phi_+(x) = \frac{1}{\sqrt{2\pi}^3} \int \frac{d^3\boldsymbol{k}}{\sqrt{2\omega_{\boldsymbol{k}}}}\, a(\boldsymbol{k}) \exp[\mathrm{i}(\boldsymbol{k}\cdot\boldsymbol{x} - \omega_{\boldsymbol{k}} t)],$$
$$\phi_-(x) = \frac{1}{\sqrt{2\pi}^3} \int \frac{d^3\boldsymbol{k}}{\sqrt{2\omega_{\boldsymbol{k}}}}\, b^+(\boldsymbol{k}) \exp[-\mathrm{i}(\boldsymbol{k}\cdot\boldsymbol{x} - \omega_{\boldsymbol{k}} t)],$$

the charge densities $\varrho_\pm = -\mathrm{i}q(\dot{\phi}^+_\pm \cdot \phi_\pm - \phi^+_\pm \cdot \dot{\phi}_\pm)$ are separately conserved, and therefore we can also identify conserved particle and anti-particle numbers

$$N_\pm = \pm\frac{Q_\pm}{q} = \pm\frac{1}{q}\int d^3\boldsymbol{x}\, \varrho_\pm(\boldsymbol{x}, t).$$

21.6a. Show that the conserved current density for QED with scalar matter (21.2) is

$$j_\mu = \mathrm{i}qc^2 \left(\partial_\mu \phi^+ \cdot \phi - \phi^+ \cdot \partial_\mu \phi + 2\mathrm{i}\frac{q}{\hbar}\phi^+ \cdot A_\mu \cdot \phi \right).$$

21.6b. Why is it not possible to derive separately conserved (anti-)particle numbers $N_{\pm}$ for the scalar particles in the interacting theory (21.2)?

21.7. Show that contrary to the case of spinor electrodynamics, it is not possible in relativistic scalar electrodynamics to derive a Coulomb gauge Hamiltonian (although Coulomb gauge can still be imposed on the Maxwell field, of course).

Why can we nevertheless find a Coulomb gauge Hamiltonian in the non-relativistic limit for the scalar fields?

Hint: The Gauss law of scalar electrodynamics in Coulomb gauge takes the form

$$\Delta\Phi = -\mathrm{i}\frac{q}{\epsilon_0}\left(\phi^+\cdot\partial_t\phi - \partial_t\phi^+\cdot\phi + 2\mathrm{i}\frac{q}{\hbar}\phi^+\Phi\phi\right).$$

21.8. Show that the junction conditions (21.28) are necessary and sufficient to ensure that the Klein-Gordon equation holds at the step of the potential.

21.9. Generalize the reasoning from Section 21.2 to the case of oblique incidence against the potential step, e.g. by considering a scalar boson running against the potential (21.21) with initial momentum components $\hbar k_x > 0$ and $\hbar k_y > 0$.

Remarks on the Solution. The *ansatz* for the Klein-Gordon wave function which complies with the boundary conditions on the incoming particle and the requirement of smoothness for all times t and values of y along the interface $x = 0$ is

$$\phi(x, y, t) = \begin{cases} [\exp(\mathrm{i}k_x x) + \beta\exp(-\mathrm{i}k_x x)]\exp[\mathrm{i}(k_y y - \omega t)], & x < 0, \\ \theta\exp[\mathrm{i}(\kappa_x x + k_y y - \omega t)], & x > 0. \end{cases}$$

The frequency follows again from the solution of the Klein-Gordon equation in the two domains,

$$\omega = c\sqrt{k_x^2 + k_y^2 + \frac{m^2c^2}{\hbar^2}} = \frac{V}{\hbar} \pm c\sqrt{\kappa_x^2 + k_y^2 + \frac{m^2c^2}{\hbar^2}}. \tag{21.134}$$

All other pertinent results follow also exactly as in Section 21.2 if we make the substitutions $k \to k_x$, $\kappa \to \kappa_x$ and $mc \to \sqrt{m^2c^2 + \hbar^2 k_y^2}$. This applies in particular also to Table 21.1 and Figure 21.1. In particular, we have generation of pairs of particles and anti-particles in the energy range

$$c\sqrt{\hbar^2 k_y^2 + m^2c^2} < \hbar\omega = c\sqrt{\hbar^2 k_x^2 + \hbar^2 k_y^2 + m^2c^2} < V - c\sqrt{\hbar^2 k_y^2 + m^2c^2}$$

if the height of the potential step satisfies

$$V > 2c\sqrt{\hbar^2 k_y^2 + m^2c^2}.$$

The wave number κ_x in this energy range is

$$\kappa_x = -\frac{1}{\hbar}\sqrt{\frac{(\hbar\omega - V)^2}{c^2} - m^2c^2 - \hbar^2 k_y^2},$$

and writing the solution for $x > 0$ as

$$\phi(x, y, t) = \theta \exp[-\mathrm{i}(-\kappa_x x - k_y y + \omega t)], \quad x > 0,$$

shows that it is an anti-particle solution with energy $\overline{E}_p = -\hbar\omega$ and momentum components $-\hbar\kappa_x > 0$, $-\hbar k_y < 0$. The kinetic+rest energy of the generated anti-particles in the region $x > 0$ is

$$K_{\overline{p}} = c\sqrt{\hbar^2\kappa_x^2 + \hbar^2 k_y^2 + m^2c^2} = V - \hbar\omega, \tag{21.135}$$

and the energy of the anti-particles is just the sum of their kinetic+rest energy and their potential energy, $\overline{E}_p = K_{\overline{p}} - V$.

21.10. Calculate the boson number operator

$$N_b = \int d^3\boldsymbol{k}\,\big(a^+(\boldsymbol{k})a(\boldsymbol{k}) + b^+(\boldsymbol{k})b(\boldsymbol{k})\big)$$

for the free Klein-Gordon field in $\boldsymbol{x}$ representation.

21.11. Show that scattering of a Klein-Gordon field off a hard sphere yields the same result (11.36) as the non-relativistic Schrödinger theory, except that the definition $k = \sqrt{2mE}/\hbar$ (where E is the kinetic energy of the scattered particle) is replaced by

$$k = \frac{1}{\hbar c}\sqrt{\hbar^2\omega^2 - m^2c^4}.$$

The hard sphere is taken into account through a boundary condition of vanishing Klein-Gordon field on the surface of the sphere, like the condition on the Schrödinger wave function in Section 11.3, i.e. we do not model it as a potential. We could think of the hard sphere in this case as arising from a hypothetical interaction which repels particles and anti-particles alike (just like gravity is equally attractive for particles and anti-particles).

21.12. You could also model an impenetrable wall for a Klein-Gordon field in the manner of the hard sphere of Problem 11. Which wave function for the Klein-Gordon field do you get if the impenetrable wall prevents the field from entering the region $x > 0$? Why does this result not contradict the Klein paradox?

21.13. Calculate the fermion number operator

$$N_f = \int d^3\boldsymbol{k} \sum_{s\in\{\downarrow,\uparrow\}} \left[b_s^+(\boldsymbol{k})b_s(\boldsymbol{k}) + d_s^+(\boldsymbol{k})d_s(\boldsymbol{k})\right]$$

for the free Dirac field in $\boldsymbol{x}$ representation.

21.14. Calculate the reflection and transmission coefficients for a Dirac field of charge q in the presence of a potential step $q\Phi(x) = V(x) = V\Theta(x)$. How do your results compare with the results for the Klein-Gordon field in Section 21.2?

21.15a. What are the non-relativistic limits of the spinor plane waves (21.72)?

21.15b. Verify the relations (21.73) for the relativistic spinor plane wave states.

21.16. Angular momentum in relativistic field theory

21.16a. Show that if $T_{\mu\nu}$ is a symmetric conserved energy momentum tensor, then the currents

$$\mathcal{M}_{\alpha\beta}{}^{\mu} = \frac{1}{c}\left(x_\alpha T_\beta{}^\mu - x_\beta T_\alpha{}^\mu\right) \tag{21.136}$$

are also conserved:

$$\partial_\mu \mathcal{M}_{\alpha\beta}{}^{\mu} = 0. \tag{21.137}$$

21.16b. The quantities $\mathcal{M}_{\alpha\beta}{}^{\mu}$ have the properties $\mathcal{M}_{\alpha\beta}{}^{0} = x_\alpha\mathcal{P}_\beta - x_\beta\mathcal{P}_\alpha$ and are therefore associated with angular momentum conservation and conservation of the center of energy motion (18.128, 18.129) in relativistic field theories. Show that invariance of the relativistic field theory

$$\begin{aligned}\mathcal{L} = &-\hbar c^2\left(\partial_\mu\phi^+ + \mathrm{i}\frac{Q}{\hbar}\phi^+ A_\mu\right)\cdot\left(\partial^\mu\phi - \mathrm{i}\frac{Q}{\hbar}A^\mu\phi\right) - \frac{m^2c^4}{\hbar}\phi^+\cdot\phi \\ &+ c\overline{\Psi}\left[\gamma^\mu\left(\frac{\mathrm{i}\hbar}{2}\overleftrightarrow{\partial}_\mu + qA_\mu\right) - mc\right]\Psi - \frac{1}{4\mu_0}F_{\mu\nu}F^{\mu\nu}.\end{aligned} \tag{21.138}$$

under rotations and Lorentz boosts

$$\epsilon^\mu = -\delta x^\mu = -\varphi^{\mu\nu}x_\nu, \quad \varphi^{\mu\nu} = -\varphi^{\nu\mu}, \tag{21.139}$$

$$\delta\phi(x) \equiv \phi'(x') - \phi(x) = 0, \quad \delta A^\mu(x) = \varphi^{\mu\nu}A_\nu(x), \tag{21.140}$$

$$\delta\Psi(x) = \frac{\mathrm{i}}{2}\varphi^{\alpha\beta}S_{\alpha\beta}\cdot\Psi(x), \quad \delta\overline{\Psi}(x) = -\frac{\mathrm{i}}{2}\varphi^{\alpha\beta}\,\overline{\Psi}(x)\cdot S_{\alpha\beta}, \tag{21.141}$$

yields the conservations laws (21.137) from the results of Section 16.2 if proper improvement terms are added. The Lorentz generators $S_{\alpha\beta}$ in the spinor representation are defined in equation (H.12).

21.16c. We have seen in the previous problem that invariance of the relativistic theory (21.138) under the rotations $\delta x^i = \varphi^{ij}x_j = \epsilon^{ijk}x_j\varphi_k$ yields densities of conserved charges $\mathcal{M}_{ij}{}^0$ which we can express in vector form through $\mathcal{M}_{ij}{}^0 = \epsilon_{ijk}\mathcal{J}_k$, $\mathcal{J}_i = \epsilon_{ijk}\mathcal{M}_{jk}{}^0/2$, i.e. $\mathcal{J} = \boldsymbol{x}\times\mathcal{P}$. On the other hand, we have seen in Problem 16.6 that the total angular momentum density $\mathcal{J}$ of non-relativistic fermions contains a spin term which is *not* proportional to any space-time coordinates x_α, and yet we have also seen in Problem 16.7 that only the *combination* of both terms in (16.26) yields the density of a conserved quantity in the presence of spin-orbit coupling. How can that be?

Replace time derivatives on spinor fields in the momentum density using the Dirac equation. This yields spin contributions to the momentum density. Show that partial integration of the resulting spin contributions to the angular momentum density yields spin terms which reduce to the spin term in equation (16.26) in the non-relativistic limit.

Solution for 16b. The electric current density for the Lagrange density (21.138) is

$$j_q^\mu = \frac{\partial\mathcal{L}}{\partial A_\mu} = -\mathrm{i}Qc^2\phi^+\left(\overleftrightarrow{\partial}^\mu - 2\mathrm{i}\frac{Q}{\hbar}A^\mu\right)\phi + qc\overline{\Psi}\gamma^\mu\Psi. \tag{21.142}$$

Addition of the identically conserved improvement term

$$-\frac{1}{\mu_0}\partial_\nu\left(x_\alpha A_\beta F^{\mu\nu}\right) = -\frac{1}{\mu_0}A_\beta F^\mu{}_\alpha - \frac{1}{\mu_0}x_\alpha\partial_\nu A_\beta\cdot F^{\mu\nu} - x_\alpha A_\beta j_q^\mu$$

to the conserved current (16.13) for the transformation (21.139–21.141) yields the gauge invariant conserved current

$$\begin{aligned} j^\mu = {} & -\varphi^{\mu\nu}x_\nu\mathcal{L} + \varphi^{\alpha\beta}x_\alpha\Bigg[\hbar c^2\left(\partial^\mu\phi^+ + \mathrm{i}\frac{Q}{\hbar}\phi^+A^\mu\right)\left(\partial_\beta\phi - \mathrm{i}\frac{Q}{\hbar}A_\beta\phi\right) \\ & + \hbar c^2\left(\partial_\beta\phi^+ + \mathrm{i}\frac{Q}{\hbar}\phi^+A_\beta\right)\left(\partial^\mu\phi - \mathrm{i}\frac{Q}{\hbar}A^\mu\phi\right) \\ & - \mathrm{i}\frac{\hbar c}{2}\,\overline{\Psi}\gamma^\mu\left(\overleftrightarrow{\partial}_\beta - 2\mathrm{i}\frac{q}{\hbar}A_\beta\right)\Psi + \frac{1}{\mu_0}F_{\beta\nu}F^{\mu\nu}\Bigg] \\ & + \varphi^{\alpha\beta}\frac{\hbar c}{4}\,\overline{\Psi}\left(\gamma^\mu S_{\alpha\beta} + S_{\alpha\beta}\gamma^\mu\right)\Psi. \end{aligned} \tag{21.143}$$

The divergence of the spinor contributions to this current density is

$$\partial_\mu j^\mu_\Psi = \varphi^{\alpha\beta}\frac{\hbar c}{4}\,\partial_\mu\left[\overline{\Psi}\left(\gamma^\mu S_{\alpha\beta}+S_{\alpha\beta}\gamma^\mu\right)\Psi\right]-\frac{c}{2}\varphi^{\alpha\beta}\overline{\Psi}\gamma_\alpha\left(\mathrm{i}\hbar\,\overset{\leftrightarrow}{\partial}_\beta+2qA_\beta\right)\Psi$$
$$-\frac{c}{2}\varphi^{\alpha\beta}x_\alpha\partial_\mu\left[\overline{\Psi}\gamma^\mu\left(\mathrm{i}\hbar\,\overset{\leftrightarrow}{\partial}_\beta+2qA_\beta\right)\Psi\right]. \tag{21.144}$$

The relation (21.85) implies that on-shell

$$\varphi^{\alpha\beta}\frac{\hbar c}{4}\,\partial_\mu\left[\overline{\Psi}\left(\gamma^\mu S_{\alpha\beta}+S_{\alpha\beta}\gamma^\mu\right)\Psi\right]-\frac{c}{2}\varphi^{\alpha\beta}\overline{\Psi}\gamma_\alpha\left(\mathrm{i}\hbar\,\overset{\leftrightarrow}{\partial}_\beta+2qA_\beta\right)\Psi=0,$$

and comparison of (21.82) and (21.86) implies that we can write the remaining part of $\partial_\mu j^\mu_\Psi$ in the form

$$\partial_\mu j^\mu_\Psi = -\frac{c}{4}\varphi^{\alpha\beta}x_\alpha\partial_\mu\left[\overline{\Psi}\gamma^\mu\left(\mathrm{i}\hbar\,\overset{\leftrightarrow}{\partial}_\beta+2qA_\beta\right)\Psi+\overline{\Psi}\gamma_\beta\left(\mathrm{i}\hbar\,\overset{\leftrightarrow}{\partial}^\mu+2qA^\mu\right)\Psi\right]$$
$$=-\frac{c}{4}\varphi^{\alpha\beta}\partial_\mu\left[x_\alpha\overline{\Psi}\gamma^\mu\left(\mathrm{i}\hbar\,\overset{\leftrightarrow}{\partial}_\beta+2qA_\beta\right)\Psi+x_\alpha\overline{\Psi}\gamma_\beta\left(\mathrm{i}\hbar\,\overset{\leftrightarrow}{\partial}^\mu+2qA^\mu\right)\Psi\right].$$

The conserved current (21.144) is therefore equivalent to the conserved current

$$j^\mu=\frac{1}{2}\varphi^{\alpha\beta}\left(x_\alpha T_\beta{}^\mu-x_\beta T_\alpha{}^\mu\right)=\frac{c}{2}\varphi^{\alpha\beta}\mathcal{M}_{\alpha\beta}{}^\mu, \tag{21.145}$$

with the symmetric stress-energy tensor for the Lagrange density (21.138) (cf. (21.87, 21.131))

$$T_\mu{}^\nu=\eta_\mu{}^\nu\mathcal{L}-\frac{c}{2}\overline{\Psi}\left[\frac{\mathrm{i}\hbar}{2}\gamma^\nu\,\overset{\leftrightarrow}{\partial}_\mu+\frac{\mathrm{i}\hbar}{2}\gamma_\mu\,\overset{\leftrightarrow}{\partial}^\nu+q\gamma^\nu A_\mu+q\gamma_\mu A^\nu\right]\Psi+\frac{1}{\mu_0}F_{\mu\lambda}F^{\nu\lambda}$$
$$+\hbar c^2\left(\partial_\mu\phi^++\mathrm{i}\frac{Q}{\hbar}\phi^+A_\mu\right)\left(\partial^\nu\phi-\mathrm{i}\frac{Q}{\hbar}A^\nu\phi\right)$$
$$+\hbar c^2\left(\partial^\nu\phi^++\mathrm{i}\frac{Q}{\hbar}\phi^+A^\nu\right)\left(\partial_\mu\phi-\mathrm{i}\frac{Q}{\hbar}A_\mu\phi\right). \tag{21.146}$$

Solution for 16c. We discuss the angular momentum densities in vector form, $\mathcal{J}_i=\epsilon_{ijk}\mathcal{M}_{jk}{}^0/2=\epsilon_{ijk}x_j\mathcal{P}_k$, with the momentum densities $\mathcal{P}_k=T_k{}^0/c$ (cf. (21.89, 21.133)),

$$\mathcal{P}=\frac{1}{2}\Psi^+\left[\frac{\hbar}{2\mathrm{i}}\overset{\leftrightarrow}{\nabla}-q\boldsymbol{A}\right]\Psi+\frac{1}{2}\overline{\Psi}\boldsymbol{\gamma}\left[\frac{\mathrm{i}\hbar}{2}\,\overset{\leftrightarrow}{\partial}_0-\frac{q}{c}\Phi\right]\Psi+\epsilon_0\boldsymbol{E}\times\boldsymbol{B}$$
$$-\hbar\left(\dot{\phi}^+-\mathrm{i}\frac{Q}{\hbar}\phi^+\Phi\right)\left(\nabla\phi-\mathrm{i}\frac{Q}{\hbar}\boldsymbol{A}\phi\right)$$
$$-\hbar\left(\nabla\phi^++\mathrm{i}\frac{Q}{\hbar}\phi^+\boldsymbol{A}\right)\left(\dot{\phi}+\mathrm{i}\frac{Q}{\hbar}\Phi\phi\right). \tag{21.147}$$

The γ matrices satisfy

$$\gamma_i \cdot \gamma_j = -\delta_{ij} \begin{pmatrix} \underline{1} & 0 \\ 0 & \underline{1} \end{pmatrix} + \frac{1}{2}\epsilon_{ijk}\epsilon_{kmn}\gamma_m \cdot \gamma_n = -\delta_{ij} \begin{pmatrix} \underline{1} & 0 \\ 0 & \underline{1} \end{pmatrix} + \frac{2}{i\hbar}\epsilon_{ijk}S_k$$

with the vector of 4×4 spin matrices $\boldsymbol{S} = i\hbar\boldsymbol{\gamma}\times\boldsymbol{\gamma}/4$, cf. (21.78). The Dirac equation then implies

$$\overline{\Psi}\boldsymbol{\gamma}\left[\frac{i\hbar}{2}\overset{\leftrightarrow}{\partial}_0 - \frac{q}{c}\Phi\right]\Psi = \Psi^+\left[\frac{\hbar}{2i}\overset{\leftrightarrow}{\nabla} - q\boldsymbol{A}\right]\Psi + \nabla\times(\Psi^+\cdot\boldsymbol{S}\cdot\Psi),$$

and we can write the momentum density in the form

$$\begin{aligned}\mathcal{P} = {} & \Psi^+\left[\frac{\hbar}{2i}\overset{\leftrightarrow}{\nabla} - q\boldsymbol{A}\right]\Psi + \frac{1}{2}\nabla\times(\Psi^+\cdot\boldsymbol{S}\cdot\Psi) + \epsilon_0\boldsymbol{E}\times\boldsymbol{B} \\ & -\hbar\left(\dot{\phi}^+ - i\frac{Q}{\hbar}\phi^+\Phi\right)\left(\nabla\phi - i\frac{Q}{\hbar}\boldsymbol{A}\phi\right) \\ & -\hbar\left(\nabla\phi^+ + i\frac{Q}{\hbar}\phi^+\boldsymbol{A}\right)\left(\dot{\phi} + i\frac{Q}{\hbar}\Phi\phi\right).\end{aligned} \tag{21.148}$$

The spin term $\mathcal{P}_S = \nabla\times(\Psi^+\cdot\boldsymbol{S}\cdot\Psi)/2$ in the momentum density contributes a term to the angular momentum of the form

$$\boldsymbol{J}_S = \int d^3x\,\boldsymbol{x}\times\frac{1}{2}[\nabla\times(\Psi^+\cdot\boldsymbol{S}\cdot\Psi)] = \int d^3x\,\Psi^+\cdot\boldsymbol{S}\cdot\Psi, \tag{21.149}$$

such that we can write the total angular momentum density also in the form

$$\mathcal{J} = \mathcal{M} + \mathcal{S}, \tag{21.150}$$

with a spin contribution $\mathcal{S} = \Psi^+\cdot\boldsymbol{S}\cdot\Psi$, and an orbital angular momentum $\mathcal{M} = \boldsymbol{x}\times\mathcal{P}_O$ with the orbital momentum density:

$$\begin{aligned}\mathcal{P}_O = {} & \Psi^+\left[\frac{\hbar}{2i}\overset{\leftrightarrow}{\nabla} - q\boldsymbol{A}\right]\Psi - \hbar\left(\dot{\phi}^+ - i\frac{Q}{\hbar}\phi^+\Phi\right)\left(\nabla\phi - i\frac{Q}{\hbar}\boldsymbol{A}\phi\right) \\ & -\hbar\left(\nabla\phi^+ + i\frac{Q}{\hbar}\phi^+\boldsymbol{A}\right)\left(\dot{\phi} + i\frac{Q}{\hbar}\Phi\phi\right) + \epsilon_0\boldsymbol{E}\times\boldsymbol{B}.\end{aligned} \tag{21.151}$$

Substitution of the non-relativistic approximations in the Dirac representation of the γ matrices (cf. (21.19, 21.97)),

$$\phi(\boldsymbol{x},t) \to \sqrt{\frac{\hbar}{2mc^2}}\phi(\boldsymbol{x},t)\exp\left(-i\frac{mc^2}{\hbar}t\right),$$

$$\Psi(\boldsymbol{x},t) = \begin{pmatrix}\psi(\boldsymbol{x},t)\\ \chi(\boldsymbol{x},t)\end{pmatrix}\exp\left(-i\frac{mc^2}{\hbar}t\right)$$

into (21.148) yields after neglecting the subleading χ components (cf. (21.100))

$$\mathcal{P}_O = \psi^+ \left[\frac{\hbar}{2\mathrm{i}} \overset{\leftrightarrow}{\nabla} - q\boldsymbol{A} \right] \psi + \phi^+ \left[\frac{\hbar}{2\mathrm{i}} \overset{\leftrightarrow}{\nabla} - Q\boldsymbol{A} \right] \phi + \epsilon_0 \boldsymbol{E} \times \boldsymbol{B} \tag{21.152}$$

and

$$\mathcal{S} = \frac{\hbar}{2} \psi^+ \cdot \underline{\boldsymbol{\sigma}} \cdot \psi. \tag{21.153}$$

If we would not have used the equations and motion and equation (21.85) to write the conserved current in the form (21.145), the spin term $\mathcal{S} = \Psi^+ \cdot \boldsymbol{S} \cdot \Psi$ would have come from the last line in equation (21.143).

21.17. New charges from local phase invariance?

We have derived expressions for charge and current densities from phase invariance

$$\delta\Psi(x) = \mathrm{i}\frac{q}{\hbar}\varphi\Psi(x), \quad \delta\Psi^+(x) = -\mathrm{i}\frac{q}{\hbar}\varphi\Psi^+(x),$$

of Lagrange densities, see e.g. (16.31, 16.32) for the charge and current densities of non-relativistic charged matter fields, and (21.142) for relativistic charged matter fields. In the final expressions we always divided out the irrelevant constant parameter φ. However, introduction of the electromagnetic potentials rendered the Lagrange densities invariant under *local* phase transformations

$$\delta\Psi(x) = \mathrm{i}\frac{q}{\hbar}\varphi(x)\Psi(x), \quad \delta\Psi^+(x) = -\mathrm{i}\frac{q}{\hbar}\varphi(x)\Psi^+(x), \quad \delta A_\mu(x) = \partial_\mu\varphi(x).$$

In this case we cannot discard the phase parameter $\varphi(x)$ from the current densities for the local symmetry. Does this provide us with additional useful notions of conserved charges for quantum electronics and quantum electrodynamics?

21.17a. Show that application of the result (16.13) to local phase transformations yields current densities

$$J^\mu = \varphi j^\mu + \frac{1}{\mu_0} F^{\mu\nu} \partial_\nu \varphi, \tag{21.154}$$

where j^μ are the current densities which were derived for constant phase parameter φ, e.g. (16.31, 16.32) or (21.142).

Show that the currents J^μ can also be written in the *strong form*[12]

$$J^\mu = \frac{1}{\mu_0} \partial_\nu \left(\varphi F^{\mu\nu} \right). \tag{21.155}$$

[12]A current J^μ is sometimes denoted as *strongly conserved* if the local conservation law $\partial_\mu J^\mu = 0$ is an identity.

21.17b. Show in particular that the charge density $\mathcal{Q}_\varphi = J^0/c$ can be written in the form

$$\mathcal{Q}_\varphi = \epsilon_0 \nabla \cdot (\varphi \boldsymbol{E}) , \tag{21.156}$$

and that the current density is

$$\boldsymbol{J} = \frac{1}{\mu_0} \nabla \times (\varphi \boldsymbol{B}) - \epsilon_0 \partial_t (\varphi \boldsymbol{E}) . \tag{21.157}$$

Apply these results to a static charge distribution $\varrho(\boldsymbol{x}) = j^0(\boldsymbol{x})/c$. The charge

$$Q_\varphi = \int d^3\boldsymbol{x}\, \mathcal{Q}_\varphi(\boldsymbol{x}, t)$$

is only conserved if Q_φ charges do not escape or enter at $|\boldsymbol{x}| \to \infty$:

$$\lim_{|\boldsymbol{x}|\to\infty} \int d^2\Omega\, |\boldsymbol{x}|\boldsymbol{x} \cdot \boldsymbol{J}(\boldsymbol{x}, t) = 0.$$

Show that this implies

$$\lim_{|\boldsymbol{x}|\to\infty} \dot{\varphi}(\boldsymbol{x}, t) = 0.$$

Show also that Q_φ differs from the standard electric charge

$$Q = \int d^3\boldsymbol{x}\, \varrho(\boldsymbol{x})$$

only by a constant factor

$$Q_\varphi = \langle \varphi \rangle Q, \tag{21.158}$$

where

$$\langle \varphi \rangle = \frac{1}{4\pi} \int d^2\Omega \lim_{|\boldsymbol{x}|\to\infty} \varphi(\boldsymbol{x}, t)$$

is the angular average of the phase parameter $\varphi(\boldsymbol{x}, t)$ at $|\boldsymbol{x}| \to \infty$.

21.18. Show for a free electron that equation (21.100) implies that a positron component ϕ in the wave function is not negligible any more relative to the electron wave function ψ at a distance of order

$$d \simeq \frac{4mc}{\hbar} \Delta x^2 \simeq 10^4\,\mathrm{nm}^{-1} \Delta x^2 = 10^{11}\,\mathrm{cm}^{-1} \Delta x^2. \tag{21.159}$$

This implies that we cannot use the wave packet for a strongly localized free electron with $\Delta x = 1$ Å beyond a distance of about 0.1 μm from the center. However, for a free electron wave packet with $\Delta x = 1$ mm the limit (21.159) is much larger than the confines of any physics or chemistry lab and therefore of no concern.

Show also that at time t, the estimate for the usable range of the wave packet is

$$d(t) \lesssim \frac{4mc}{\hbar}\Delta x(0)\Delta x(t). \tag{21.160}$$

21.19. Show that the Foldy-Wouthuysen transformation (21.111) can also be written as

$$|\Upsilon_{FWT}(t)\rangle = \exp[F(t) + W(t) + T(t) + C(t) + \mathcal{O}(\mathcal{E}/mc^2)^4]|\Upsilon(t)\rangle,$$

with

$$C(t) = \frac{q\hbar}{16m^3c^4}\gamma^0\big(\hbar\nabla\cdot\boldsymbol{E}(\mathbf{x},t) + 2\mathrm{i}\boldsymbol{E}(\mathbf{x},t)\cdot[\mathbf{p} - q\boldsymbol{A}(\mathbf{x},t)]\big)$$
$$+\,\mathrm{i}\frac{q\hbar^2}{16m^3c^4}\big(\nabla\times\boldsymbol{E}(\mathbf{x},t)\big)\cdot\begin{pmatrix}\underline{\boldsymbol{\sigma}} & \underline{0}\\ \underline{0} & -\underline{\boldsymbol{\sigma}}\end{pmatrix}.$$

21.20. We have derived the equations (12.21, 12.23) for particles which satisfy the relativistic dispersion equation. In the meantime, we have seen that at the quantum level these particles are described by scalar fields ϕ, spinors ψ, or vector fields A_μ. The factor g counts spin and internal symmetry degrees of freedom and has the form $g = g_s \times d_{\mathrm{rep}(G)}$, where $d_{\mathrm{rep}(G)}$ is the dimension of the representation of the internal symmetry group G under which the fields transform.

21.20a. Scalar fields have $g_s = 1$. Show that in $d + 1$ space-time dimensions, $g_s = 2^{\lfloor (d-1)/2\rfloor}$ for Dirac fields and $g_s = d - 1$ for vector fields.

Hint: A Dirac spinor in $d + 1$ space-time dimensions has $2^{\lfloor (d+1)/2\rfloor}$ components, see Appendix G (note that there d denotes the number of space-time dimensions).

21.20b. We have seen that scalar fields can be either real or complex (and similar remarks apply to spinor and vector fields if we go beyond quantum electrodynamics into the standard model of particle physics). However, a complex field has twice as many degrees of freedom as a real field. Should g therefore not include an additional factor g_c with $g_c = 2$ for complex fields and $g_c = 1$ for real fields?

21.21. Formulate the basic relations for basis kets $|x,\mu\rangle$, $|k,\alpha\rangle$ for the potentials $|A_D\rangle$ in Lorentz gauge in analogy to the corresponding relations (18.24–18.27) in Coulomb gauge.

21.22. Show that the two representations given in equation (21.130) for the gauge transformation function $g(\boldsymbol{x}, t)$ are indeed equivalent (hint: use the fact that $A^{\mu}(x)$ satisfies the Gauss law $\nabla \cdot \boldsymbol{E} = \varrho/\epsilon_0$).

Show also that the gauge transformation (21.129, 21.130) takes us from any vector potential $A_{\mu}(x)$ which satisfies Maxwell's equations into the vector potential in Coulomb gauge.