

# Dirac and Klein-Gordon particles in external fields

## 1 Introduction

In relativistic quantum mechanics free particles are described by wave equations: the Klein–Gordon equation for particles without spin and the Dirac equation for particles with spin  $\frac{1}{2}$ . If the particles move in external electromagnetic fields, generated by classical sources, the interaction of these fields and the particles is described by adding appropriate terms to the wave equations. If one wants to confine oneself to single particle theories the electromagnetic fields should change relatively slowly in space and time so as to avoid effects due to particle production.

The purpose of this chapter is to find equations of motion and of spin for Klein–Gordon and Dirac particles of what one may call the Ehrenfest type, i.e. expressions for the time derivatives of the expectation values of the position and spin operators. The latter will be uniquely determined by imposing their transformation character with respect to the Poincaré group. The Hamiltonian, which governs the time behaviour of the expectation values, will be brought into a form which allows to distinguish between positive- and negative-energy solutions; it will be given up to terms with the first derivatives of the potentials (the fields).

In sections 2 and 3 the equations of motion and of spin for a particle with spin  $\frac{1}{2}$  are derived<sup>1</sup>. They will turn out to have forms analogous to those found in chapter IV for a classical composite particle with inner angular momentum. For composite particles without inner angular momentum the equations of that chapter simplify considerably. In sections 4 and 5 it will appear that equations of that simple type may indeed be derived for a quantum particle without spin, i.e. a particle described by the equation of Klein and Gordon.

<sup>1</sup> L. G. Sutorp and S. R. de Groot, N. Cim. **65A**(1970)245, on which paper the discussion in these sections will be based.

## 2 The free Dirac particle

### a. Invariances of the Dirac equation

It is useful to study first the free particle case, since it contains a number of aspects which it has in common with the problem of a particle in a field.

In Dirac's theory for a single particle the states are described by four-component wave functions  $\psi(\mathbf{R}, t)$  that depend on space and time in the coordinate representation. The time evolution of these wave functions is governed by the Dirac equation. This equation may be written as

$$H_{\text{op}}\psi(\mathbf{R}, t) = -\frac{\hbar}{i} \frac{\partial \psi(\mathbf{R}, t)}{\partial t}, \quad (1)$$

where the Hamilton operator for a free particle with mass  $m (\neq 0)$  is given by

$$H_{\text{op}} = c\boldsymbol{\alpha} \cdot \mathbf{P}_{\text{op}} + \beta mc^2. \quad (2)$$

The symbols  $\boldsymbol{\alpha}$  and  $\beta$  stand for hermitian  $4 \times 4$  matrices which obey the anti-commutation rules

$$\{\boldsymbol{\alpha}, \boldsymbol{\alpha}\} = 2\mathbf{U}, \quad \{\boldsymbol{\alpha}, \beta\} = 0, \quad \{\beta, \beta\} = 2. \quad (3)$$

(where  $\mathbf{U}$  is the unit tensor and 2 stands for twice the unit  $4 \times 4$  matrix). Furthermore  $\mathbf{P}_{\text{op}}$  is the momentum operator, which reads

$$\mathbf{P}_{\text{op}} = \frac{\hbar}{i} \frac{\partial}{\partial \mathbf{R}} \quad (4)$$

in the coordinate representation.

Physical quantities are represented by operators acting on wave functions. The expectation value of an operator  $\Omega_{\text{op}}$  (which is a function of the coordinate  $\mathbf{R}$  and the momentum operator  $(\hbar/i)\partial/\partial \mathbf{R}$ ) in a state characterized by a wave function  $\psi(\mathbf{R}, t)$  is defined as

$$\bar{\Omega}_{\text{op}} = \int \psi^\dagger(\mathbf{R}, t) \Omega_{\text{op}} \left( \mathbf{R}, \frac{\hbar}{i} \frac{\partial}{\partial \mathbf{R}} \right) \psi(\mathbf{R}, t) d\mathbf{R}. \quad (5)$$

The Dirac equation (1) with (2) is covariant under the transformations of the Poincaré group, of which we shall study in particular spatial translations, spatial rotations, spatial inversions, time reversal and pure Lorentz transformations.

In a coordinate frame which is connected to the original frame by an infinitesimal translation

$$\begin{aligned} \mathbf{R}' &= \mathbf{R} + \boldsymbol{\varepsilon}, \\ t' &= t, \end{aligned} \quad (6)$$

(where  $\boldsymbol{\varepsilon}$  is an infinitesimal vector), the wave function transforms as

$$\psi'(\mathbf{R}', t') = \psi(\mathbf{R}, t), \quad (7)$$

since then it follows that (1) with (2) is invariant, i.e. valid for quantities with primes throughout. Moreover the inner product  $\int \psi_1^\dagger \psi_2 d\mathbf{R}$  of two wave functions is invariant under this transformation.

The expectation value in the new coordinate frame

$$\int \psi'^\dagger(\mathbf{R}', t') \Omega_{\text{op}} \left( \mathbf{R}', \frac{\hbar}{i} \frac{\partial}{\partial \mathbf{R}'} \right) \psi'(\mathbf{R}', t') d\mathbf{R}' \quad (8)$$

may be written (up to first order in  $\boldsymbol{\varepsilon}$ ) as

$$\begin{aligned} &\int \psi^\dagger(\mathbf{R}', t) \Omega_{\text{op}} \left( \mathbf{R}', \frac{\hbar}{i} \frac{\partial}{\partial \mathbf{R}'} \right) \psi(\mathbf{R}', t) d\mathbf{R}' \\ &+ \boldsymbol{\varepsilon} \cdot \int \psi^\dagger(\mathbf{R}', t) \left[ \frac{\partial}{\partial \mathbf{R}'}, \Omega_{\text{op}} \left( \mathbf{R}', \frac{\hbar}{i} \frac{\partial}{\partial \mathbf{R}'} \right) \right] \psi(\mathbf{R}', t) d\mathbf{R}', \end{aligned} \quad (9)$$

where a partial integration has led to a commutator. We shall write this as

$$\bar{\Omega}_{\text{op}} + \bar{\delta} \bar{\Omega}_{\text{op}}, \quad (10)$$

where the first term is equal to (5). The second is the expectation value of the operator

$$\delta \Omega_{\text{op}} = \frac{i}{\hbar} \boldsymbol{\varepsilon} \cdot [\mathbf{P}_{\text{op}}, \Omega_{\text{op}}]. \quad (11)$$

This shows that  $\mathbf{P}_{\text{op}}$  is the generator of spatial translations.

A coordinate frame which is related to the original frame by an infinitesimal rotation has coordinates

$$\begin{aligned} \mathbf{R}' &= \mathbf{R} + \boldsymbol{\varepsilon} \wedge \mathbf{R}, \\ t' &= t, \end{aligned} \quad (12)$$

with  $\boldsymbol{\varepsilon}$  an infinitesimal vector. The wave function in the new frame is

$$\psi'(\mathbf{R}', t') = (1 - \frac{1}{2} i \boldsymbol{\varepsilon} \cdot \boldsymbol{\sigma}) \psi(\mathbf{R}, t), \quad (13)$$

where the matrix  $\sigma$  is defined as

$$\sigma = -\frac{1}{2}i\alpha \wedge \alpha. \quad (14)$$

Indeed one may check that the transformations (12) and (13) leave the Dirac equation (1) with (2) and the inner product of two wave functions invariant.

The expectation value of an operator  $\Omega_{\text{op}}$  in the new coordinate frame becomes, upon introduction of (12) and (13) into (8), of the form (10) with the operator

$$\delta\Omega_{\text{op}} = \frac{i}{\hbar} \varepsilon^i [\mathbf{R} \wedge \mathbf{P}_{\text{op}} + \frac{1}{2}\hbar\sigma, \Omega_{\text{op}}]. \quad (15)$$

This shows that  $\mathbf{R} \wedge \mathbf{P}_{\text{op}} + \frac{1}{2}\hbar\sigma$  is the generator of spatial rotations.

A vector operator is characterized by

$$\delta\Omega_{\text{op}} = \varepsilon \wedge \Omega_{\text{op}}, \quad (16)$$

(cf. (12)). For such operators (15) becomes

$$[(\mathbf{R} \wedge \mathbf{P}_{\text{op}} + \frac{1}{2}\hbar\sigma)^i, \Omega_{\text{op}}^j] = i\hbar\varepsilon^{ijk}\Omega_{k,\text{op}}, \quad (17)$$

with  $\varepsilon^{ijk}$  the Levi-Civita symbol.

For *spatial inversion*

$$\begin{aligned} \mathbf{R}' &= -\mathbf{R}, \\ t' &= t \end{aligned} \quad (18)$$

the wave function transforms as<sup>1</sup>

$$\psi'(\mathbf{R}', t') = \beta\psi(\mathbf{R}, t). \quad (19)$$

Indeed (18) and (19) leave the Dirac equation (1) with (2) and the inner product invariant.

The expectation value of an operator  $\Omega_{\text{op}}$  in the new frame reads:

$$\begin{aligned} \int \psi'^{\dagger}(\mathbf{R}', t')\Omega_{\text{op}}\left(\mathbf{R}', \frac{\hbar}{i}\frac{\partial}{\partial\mathbf{R}'}\right)\psi'(\mathbf{R}', t')d\mathbf{R}' \\ = \int \psi^{\dagger}(\mathbf{R}, t)\beta\Omega_{\text{op}}\left(-\mathbf{R}, -\frac{\hbar}{i}\frac{\partial}{\partial\mathbf{R}}\right)\beta\psi(\mathbf{R}, t)d\mathbf{R}. \end{aligned} \quad (20)$$

A polar or axial vector operator is characterized by the property that the expectation value in the new frame is equal to minus or plus the expectation

<sup>1</sup> Phase factors will be left out since they do not affect the expectation values considered here.

value in the old frame. Hence it follows from (20) that polar or axial vector operators satisfy the relation

$$\Omega_{\text{op}}(-\mathbf{R}, -\mathbf{P}_{\text{op}}) = \mp\beta\Omega_{\text{op}}(\mathbf{R}, \mathbf{P}_{\text{op}})\beta. \quad (21)$$

For *time inversion*

$$\begin{aligned} \mathbf{R}' &= \mathbf{R}, \\ t' &= -t \end{aligned} \quad (22)$$

the wave function transforms as

$$\psi'(\mathbf{R}', t') = T\psi^*(\mathbf{R}, t), \quad (23)$$

where the asterisk indicates the complex conjugate. The matrix  $T$  is such that it transforms the Dirac matrices in the following way:

$$T^{-1}\alpha T = -\alpha^*, \quad T^{-1}\beta T = \beta^*. \quad (24)$$

From these relations it follows that  $T^*T$  is a multiple  $\lambda$  of the  $4 \times 4$  unit matrix. The anti-linear transformation (23) with (22) and (24) leaves the Dirac equation (1) with (2) invariant. The inner product of two wave functions changes into its complex conjugate, so that its absolute value remains the same.

The expectation value of an operator  $\Omega_{\text{op}}$  in the new frame is

$$\begin{aligned} \int \psi'^{\dagger}(\mathbf{R}', t')\Omega_{\text{op}}\left(\mathbf{R}', \frac{\hbar}{i}\frac{\partial}{\partial\mathbf{R}'}\right)\psi'(\mathbf{R}', t')d\mathbf{R}' \\ = \int \psi^{\dagger}(\mathbf{R}, t)\tilde{T}\tilde{\Omega}_{\text{op}}\left(\mathbf{R}, -\frac{\hbar}{i}\frac{\partial}{\partial\mathbf{R}}\right)T^*\psi(\mathbf{R}, t)d\mathbf{R}, \end{aligned} \quad (25)$$

as follows by inserting (23) in the first member and taking the transpose, which is denoted by a tilde. Choosing for  $\Omega_{\text{op}}$  the unit operator and requiring the normalization of the wave function to be invariant one finds that the matrix  $T$  is unitary ( $T^{\dagger}T = 1$ ). From this property together with  $T^*T = \lambda$  it follows that  $\tilde{T} = \pm T$  and also  $T^* = \pm T^{-1}$ . Thus instead of (25) one may write

$$\begin{aligned} \int \psi'^{\dagger}(\mathbf{R}', t')\Omega_{\text{op}}\left(\mathbf{R}', \frac{\hbar}{i}\frac{\partial}{\partial\mathbf{R}'}\right)\psi'(\mathbf{R}', t')d\mathbf{R}' \\ = \int \psi^{\dagger}(\mathbf{R}, t)T\tilde{\Omega}_{\text{op}}\left(\mathbf{R}, -\frac{\hbar}{i}\frac{\partial}{\partial\mathbf{R}}\right)T^{-1}\psi(\mathbf{R}, t)d\mathbf{R}. \end{aligned} \quad (26)$$

We now turn to the discussion of *pure Lorentz transformations*. Under an

infinitesimal pure Lorentz transformation the space–time coordinates transform according to

$$\begin{aligned} \mathbf{R}' &= \mathbf{R} - \varepsilon c t, \\ c t' &= c t - \varepsilon \cdot \mathbf{R}, \end{aligned} \quad (27)$$

with  $\varepsilon$  an infinitesimal vector. The wave function then transforms as

$$\psi'(\mathbf{R}', t') = (1 - \frac{1}{2}\varepsilon \cdot \boldsymbol{\alpha})\psi(\mathbf{R}, t), \quad (28)$$

since the Dirac equation (1) with (2) and the inner product is invariant for the transformation (27–28).

We now want to compare the expectation value (5) of an operator  $\Omega_{\text{op}}$  at the time  $t$  with an expectation value (8) at the time  $t'$ , which is numerically equal to  $t$ :

$$\int \psi'^{\dagger}(\hat{\mathbf{R}}', t') \Omega_{\text{op}} \left( \hat{\mathbf{R}}', \frac{\hbar}{i} \frac{\partial}{\partial \hat{\mathbf{R}}'} \right) \psi'(\hat{\mathbf{R}}', t') d\mathbf{R}'. \quad (29)$$

Here the variables  $\hat{\mathbf{R}}'$  and  $t'$  occur, which correspond to the variables  $\hat{\mathbf{R}}$  and  $t$  in the old frame. The latter follow from the inverse of the Lorentz transformation (27). One has, with  $t' = t$ :

$$\begin{aligned} \hat{\mathbf{R}} &= \hat{\mathbf{R}}' + \varepsilon c t, \\ c t &= c t + \varepsilon \cdot \hat{\mathbf{R}}', \end{aligned} \quad (30)$$

up to first order in  $\varepsilon$ . From (28) with circumflexes, i.e. from

$$\psi'(\hat{\mathbf{R}}', t') = (1 - \frac{1}{2}\varepsilon \cdot \boldsymbol{\alpha})\psi(\hat{\mathbf{R}}, t) \quad (31)$$

and (30) it follows with the Dirac equation (1) that one has:

$$\begin{aligned} \psi'(\hat{\mathbf{R}}', t') &= \psi(\hat{\mathbf{R}}, t) - \frac{1}{2}\varepsilon \cdot \boldsymbol{\alpha} \psi(\hat{\mathbf{R}}, t) \\ &+ c t \varepsilon \cdot \frac{\partial \psi(\hat{\mathbf{R}}, t)}{\partial \hat{\mathbf{R}}'} - \frac{i}{\hbar c} \varepsilon \cdot \hat{\mathbf{R}}' H_{\text{op}} \left( \hat{\mathbf{R}}', \frac{\hbar}{i} \frac{\partial}{\partial \hat{\mathbf{R}}'} \right) \psi(\hat{\mathbf{R}}, t). \end{aligned} \quad (32)$$

Inserting this expression and its hermitian conjugate into (29) we obtain as the expectation value in the new coordinate frame an expression of the form (10) with

$$\delta \Omega_{\text{op}} = \frac{i}{\hbar} \varepsilon \cdot [N_{\text{op}} - c t \mathbf{P}_{\text{op}}, \Omega_{\text{op}}], \quad (33)$$

where we introduced the abbreviation

$$N_{\text{op}} \equiv c^{-1} \mathbf{R} H_{\text{op}} - \frac{1}{2} i \hbar \boldsymbol{\alpha} \quad (34)$$

or, with the use of (2),

$$N_{\text{op}} = \frac{1}{2} c^{-1} \{ \mathbf{R}, H_{\text{op}} \}, \quad (35)$$

where the curly brackets indicate the anticommutator. In this way we found that  $N_{\text{op}} - c t \mathbf{P}_{\text{op}}$  is the generator of pure Lorentz transformations.

### b. Covariance requirements on position and spin

For the description of the behaviour of the particle we need operators for the position and for the spin. A number of constraints upon these operators will follow from requirements about their transformation properties with respect to the Poincaré group, in particular with respect to spatial translations, spatial rotations, spatial inversions, time reversal and pure Lorentz transformations.

As transformation properties with respect to infinitesimal translations (6) we require that the expectation value of the position operator  $X_{\text{op}}$  change by an amount  $\varepsilon$  and that that of the spin operator  $s_{\text{op}}$  be invariant. Then from (11) it follows that

$$[\mathbf{P}_{\text{op}}, X_{\text{op}}] = \frac{\hbar}{i} \mathbf{U}, \quad (36)$$

$$[\mathbf{P}_{\text{op}}, s_{\text{op}}] = 0. \quad (37)$$

As to the rotation properties we require that both the position and spin operator be vectors, so that one has from (17)

$$[(\mathbf{R} \wedge \mathbf{P}_{\text{op}} + \frac{1}{2} \hbar \boldsymbol{\sigma})^i, X_{\text{op}}^j] = i \hbar \varepsilon^{ijk} X_{k,\text{op}}, \quad (38)$$

$$[(\mathbf{R} \wedge \mathbf{P}_{\text{op}} + \frac{1}{2} \hbar \boldsymbol{\sigma})^i, s_{\text{op}}^j] = i \hbar \varepsilon^{ijk} s_{k,\text{op}}. \quad (39)$$

As regards the transformation properties with respect to spatial inversion we postulate that the position operator be a polar vector and the spin operator an axial vector. In view of (21) this means that we require

$$X_{\text{op}}(-\mathbf{R}, -\mathbf{P}_{\text{op}}) = -\beta X_{\text{op}}(\mathbf{R}, \mathbf{P}_{\text{op}}) \beta, \quad (40)$$

$$s_{\text{op}}(-\mathbf{R}, -\mathbf{P}_{\text{op}}) = \beta s_{\text{op}}(\mathbf{R}, \mathbf{P}_{\text{op}}) \beta. \quad (41)$$

For the transformation property with respect to time reversal we require that the expectation value of the position operator be invariant, while that of the spin operator should change sign. In view of (26) this means that we postulate

$$X_{\text{op}}(\mathbf{R}, -\mathbf{P}_{\text{op}}) = T \tilde{X}_{\text{op}}(\mathbf{R}, \mathbf{P}_{\text{op}}) T^{-1}, \quad (42)$$

$$s_{\text{op}}(\mathbf{R}, -\mathbf{P}_{\text{op}}) = -T \tilde{s}_{\text{op}}(\mathbf{R}, \mathbf{P}_{\text{op}}) T^{-1}, \quad (43)$$

where the tilde indicates the transposed of a  $4 \times 4$  matrix.

We now turn to a discussion of the transformation properties of the position and spin operators under pure Lorentz transformations. The expectation value of the position operator  $X_{op}$  will be required to change under the infinitesimal pure Lorentz transformation (27) by an amount<sup>1</sup> which is equal to the expectation value of the operator

$$\delta X_{op} = -\varepsilon ct + \frac{i}{2\hbar c} \{\varepsilon \cdot X_{op}, [H_{op}, X_{op}]\}. \quad (44)$$

Therefore it follows from (10) with (33) that the covariance condition<sup>2</sup> for the position operator is:

$$[N_{op}^i, X_{op}^j] = \frac{1}{2}c^{-1}\{X_{op}^i, [H_{op}, X_{op}^j]\}, \quad (45)$$

where (36) has been employed. The use of the latter formula had as a consequence that the terms with the time  $t$  cancelled, so that the requirement (45) contains only the three-vector  $X_{op}$  for the position operator.

For the spin operator  $s_{op}$  we require that its expectation value change under the pure Lorentz transformation (27) by a term<sup>3</sup> which is the expectation

<sup>1</sup> In the classical theory of a composite particle the set of centres of energy at successive times determines a world line independent of the Lorentz frame. As a result the positions observed in different Lorentz frames are connected in a particular way (cf. M. H. L. Pryce, Proc. Roy. Soc. A **195**(1949)62). In fact, let us consider the two points  $t, X(t)$  and  $\bar{t}, X(\bar{t})$  on the world line of which the time coordinates  $t$  in the reference frame and  $\bar{t}$  in an infinitesimally different frame have the same numerical value. Thus from (27),  $t \equiv \bar{t} = \bar{t} - c^{-1}\varepsilon \cdot X(\bar{t})$  and  $X'(t) \equiv X'(\bar{t}) = X(\bar{t}) - \varepsilon c\bar{t}$ . From the first of these equations one has up to first order in  $\varepsilon$  that  $c\bar{t} = ct + \varepsilon \cdot X(t)$ . With the help of this relation the second equation becomes upon Taylor expansion up to first order

$$X'(t) - X(t) = -\varepsilon ct + c^{-1}\varepsilon \cdot X(t) \frac{dX(t)}{dt}.$$

This expression is equal to the expectation value of (44) for a narrow wave packet in the limit  $\hbar \rightarrow 0$ , since then the expectation value of a (symmetrized) product of operators is equal to the product of expectation values.

<sup>2</sup> Cf. T. F. Jordan and N. Mukunda, Phys. Rev. **132**(1963)1842; G. Lugarini and M. Pauri, N. Cim. **47A**(1967)299.

<sup>3</sup> In the classical theory of a composite particle the inner angular momentum  $s$  is the space-space part ( $s^{23}, s^{31}, s^{12}$ ) of an antisymmetric tensor  $s^{\alpha\beta}$  of which the space-time components ( $s^{10}, s^{20}, s^{30}$ ) are denoted as  $t$ . With the same notation as used above we find that in a Lorentz frame which is connected to the observer's frame by an infinitesimal Lorentz transformation, the inner angular momentum  $s'$  at the time  $\bar{t}$  which is numerically equal to  $t$  is  $s'(t) = s(\bar{t}) + \varepsilon \wedge t(\bar{t})$ . With a Taylor expansion this relation becomes

$$s'(t) - s(t) = \varepsilon \wedge t(t) + c^{-1}\varepsilon \cdot X(t) \frac{ds(t)}{dt}.$$

value of the operator

$$\delta s_{op} = \varepsilon \wedge t_{op} + \frac{i}{2\hbar c} \{\varepsilon \cdot X_{op}, [H_{op}, s_{op}]\} \quad (46)$$

with the three-vector operator  $t_{op}$  such that

$$\delta t_{op} = -\varepsilon \wedge s_{op} + \frac{i}{2\hbar c} \{\varepsilon \cdot X_{op}, [H_{op}, t_{op}]\}. \quad (47)$$

With (10) and (33) it now follows that the covariance condition for the spin operator is

$$[N_{op}^i, s_{op}^j] = \frac{1}{2}c^{-1}\{X_{op}^i, [H_{op}, s_{op}^j]\} + i\hbar\varepsilon^{ijk}t_{k,op} \quad (48)$$

together with the relation

$$[N_{op}^i, t_{op}^j] = \frac{1}{2}c^{-1}\{X_{op}^i, [H_{op}, t_{op}^j]\} - i\hbar\varepsilon^{ijk}s_{k,op}, \quad (49)$$

where (37), which is valid both for  $s_{op}$  and  $t_{op}$ , has been used.

The conditions (36–43), (45) and (48–49) will be employed for the determination of the form of the position and spin operators.

### c. Transformation of the Hamiltonian to even form; the position and spin operators

In the Pauli representation the Dirac matrices  $\alpha$  and  $\beta$  of the Hamilton operator (2) are written as

$$\alpha = \rho_1 \sigma, \quad \beta = \rho_3, \quad (50)$$

where the matrices  $\sigma$  are the  $4 \times 4$  matrices

$$\sigma = \begin{pmatrix} \tau & 0 \\ 0 & \tau \end{pmatrix} \quad (51)$$

with  $\tau$  the  $2 \times 2$  Pauli matrices

$$\tau_1, \tau_2, \tau_3 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (52)$$

Likewise one finds

$$t'(t) - t(t) = -\varepsilon \wedge s(t) + c^{-1}\varepsilon \cdot X(t) \frac{dt(t)}{dt}.$$

For narrow wave packets in the limit  $\hbar \rightarrow 0$  one finds that these expressions are the expectation values of (46) and (47).

The matrices  $\rho$  are the  $4 \times 4$  matrices:

$$\rho_1, \rho_2, \rho_3 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad (53)$$

where 1 stands for the  $2 \times 2$  unit matrix. (The advantage of the use of  $\rho$ - and  $\sigma$ -matrices is that the three  $\rho$ -matrices commute with the three  $\sigma$ -matrices, while the product rules for the  $\rho$ -matrices and for the  $\sigma$ -matrices amongst each other are the same as those for the Pauli matrices  $\tau$ .) The Dirac matrices (50) are thus of the form:

$$\alpha = \begin{pmatrix} 0 & \tau \\ \tau & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (54)$$

The Dirac equation (1) with (2) may now be written as a set of two equations for the upper two and lower two components  $\psi_1$  and  $\psi_2$  of the four-component wave function  $\psi$ :

$$\begin{aligned} c\tau \cdot \mathbf{P}_{\text{op}} \psi_2 + mc^2 \psi_1 &= -\frac{\hbar}{i} \frac{\partial \psi_1}{\partial t}, \\ c\tau \cdot \mathbf{P}_{\text{op}} \psi_1 - mc^2 \psi_2 &= -\frac{\hbar}{i} \frac{\partial \psi_2}{\partial t}. \end{aligned} \quad (55)$$

These equations are coupled because the matrices  $\alpha$ , which occur in the Hamilton operator, have ‘odd’ character in the representation (54), i.e. they couple the upper and lower components of the wave function  $\psi$ . The equations for upper and lower components may be uncoupled by performing a unitary transformation due to Pryce<sup>1</sup> and Foldy–Wouthuysen<sup>2</sup>:

$$U_{\text{op}} \equiv \frac{E_{\text{op}} + mc^2 + c\beta\alpha \cdot \mathbf{P}_{\text{op}}}{\{2E_{\text{op}}(E_{\text{op}} + mc^2)\}^{\frac{1}{2}}} \quad (56)$$

with the abbreviation

$$E_{\text{op}} \equiv (c^2 \mathbf{P}_{\text{op}}^2 + m^2 c^4)^{\frac{1}{2}}. \quad (57)$$

(One may find the expression (56) by solving the eigenvalue problem of the Hamiltonian (2) and using the complex conjugates of the eigenvectors as the rows of the matrix  $U_{\text{op}}$ .)

Indeed with the transformation (56) the Hamilton operator becomes

$$\hat{H}_{\text{op}} \equiv U_{\text{op}} H_{\text{op}} U_{\text{op}}^\dagger = \beta E_{\text{op}}, \quad (58)$$

<sup>1</sup> M. H. L. Pryce, Proc. Roy. Soc. A195(1949)62.

<sup>2</sup> L. L. Foldy and S. A. Wouthuysen, Phys. Rev. 78(1950)29.

which has ‘even’ form, since  $\beta$  has ‘even’ character. The circumflex will be employed to indicate operators in the Pryce–Foldy–Wouthuysen (P–FW) picture in order to distinguish them from the original operators in the Dirac picture.

Since now the Hamilton operator has the simple form (58) its eigenvalues are immediately seen to be  $\pm(c^2 \mathbf{p}^2 + m^2 c^4)^{\frac{1}{2}}$  with  $\mathbf{p}$  the eigenvalue of the momentum operator  $\mathbf{P}_{\text{op}}$ . The positive- and negative-energy eigenfunctions have now the property that the lower two or upper two components vanish.

If one calculates the expectation value of a physical quantity for a positive- or a negative-energy solution only the part of the corresponding operator that is even in the P–FW picture plays a role. In particular if one wants to define the *position operator* only its ‘even’ part is of importance. This even part, which we shall simply denote by the symbol  $X_{\text{op}}$  from now on, is completely determined if we impose a number of conditions. In the first place, from the transformation properties of translation (36), rotation (38), spatial inversion (40) and time reversal (42) with  $T = \sigma_2$  in the Pauli representation<sup>1</sup> it follows that in the P–FW picture  $X_{\text{op}}$  has the form

$$\hat{X}_{\text{op}} \equiv U_{\text{op}} X_{\text{op}} U_{\text{op}}^\dagger = \mathbf{R} + \{f_1(E_{\text{op}}) + \beta f_2(E_{\text{op}})\} \boldsymbol{\sigma} \wedge \mathbf{P}_{\text{op}}, \quad (59)$$

where  $f_1(E_{\text{op}})$  and  $f_2(E_{\text{op}})$  are arbitrary real functions of  $E_{\text{op}}$ . Indeed  $\mathbf{P}_{\text{op}}$  and  $\boldsymbol{\sigma}$  are the only vectors available and hence  $\mathbf{P}_{\text{op}}$  and  $\boldsymbol{\sigma} \wedge \mathbf{P}_{\text{op}}$  the only polar vectors. If one limits oneself to vectors that have the right transformation character under time reversal one is left with  $\boldsymbol{\sigma} \wedge \mathbf{P}_{\text{op}}$  only<sup>2</sup>.

The transformation character under pure Lorentz transformations is determined by the commutation rule (45), which reads in the P–FW picture

$$[\hat{N}_{\text{op}}^i, \hat{X}_{\text{op}}^j] = \frac{1}{2} c^{-1} [\hat{X}_{\text{op}}^i, [\hat{H}_{\text{op}}, \hat{X}_{\text{op}}^j]]. \quad (60)$$

The left-hand side contains the generator  $\hat{N}_{\text{op}}$  in the P–FW picture. It has been given in (35) in the Dirac picture. In the P–FW picture the Hamiltonian  $\hat{H}_{\text{op}}$  is given by (58) while the Dirac coordinate gets the form

$$\hat{\mathbf{R}}_{\text{op}} \equiv U_{\text{op}} \mathbf{R} U_{\text{op}}^\dagger = \mathbf{R} + \boldsymbol{\xi}_{\text{op}}, \quad (61)$$

where

$$\boldsymbol{\xi}_{\text{op}} \equiv \frac{\hbar}{i} \frac{\partial U_{\text{op}}}{\partial \mathbf{P}_{\text{op}}} U_{\text{op}}^\dagger = -\frac{\hbar}{i} U_{\text{op}} \frac{\partial U_{\text{op}}^\dagger}{\partial \mathbf{P}_{\text{op}}} \equiv \boldsymbol{\xi}_{e,\text{op}} + \boldsymbol{\xi}_{o,\text{op}}. \quad (62)$$

<sup>1</sup> The  $T$ -matrix may be chosen as  $\sigma_2$  in the Pauli representation (50), as follows from (24). Indeed  $\sigma_2$  fulfils the relations  $T^* T = \lambda$  and  $T^\dagger T = 1$ , with  $\lambda = -1$ .

<sup>2</sup> If one does not impose time reversal invariance from the beginning one should write additional terms  $\{f_3(E_{\text{op}}) + \beta f_4(E_{\text{op}})\} \mathbf{P}_{\text{op}}$  in (59). If the requirement (60) is imposed on (59) with these terms added one finds that  $f_3(E_{\text{op}})$  and  $f_4(E_{\text{op}})$  vanish. Hence, strictly spoken, time reversal invariance need not be invoked to obtain a unique position operator. The latter is also true for the obtention of the spin operator.

The explicit forms for the even and odd parts  $\xi_{e,op}$  and  $\xi_{o,op}$  follow with (56)

$$\begin{aligned}\xi_{e,op} &= \frac{\hbar c^2 \mathbf{P}_{op} \wedge \boldsymbol{\sigma}}{2E_{op}(E_{op} + mc^2)}, \\ \xi_{o,op} &= -\frac{\hbar ic \boldsymbol{\beta} \boldsymbol{\alpha}}{2E_{op}} + \frac{\hbar ic^3 \boldsymbol{\beta} \boldsymbol{\alpha} \cdot \mathbf{P}_{op} \mathbf{P}_{op}}{2E_{op}^2(E_{op} + mc^2)}.\end{aligned}\quad (63)$$

The generator  $\hat{N}_{op}$  in the P-FW picture becomes now:

$$\hat{N}_{op} = \frac{1}{2} c^{-1} \boldsymbol{\beta} \{ \mathbf{R}, E_{op} \} + \frac{\beta \hbar c \mathbf{P}_{op} \wedge \boldsymbol{\sigma}}{2(E_{op} + mc^2)}.\quad (64)$$

If (59) and (64) are inserted into (60) one obtains the result that a certain linear combination of the independent tensors

$$P_{op}^i (\boldsymbol{\sigma} \wedge \mathbf{P}_{op})^j, \quad P_{op}^j (\boldsymbol{\sigma} \wedge \mathbf{P}_{op})^i, \quad \varepsilon^{ijk} \sigma_k \quad (65)$$

vanishes. The tensor  $\varepsilon^{ijk} P_{k,op} \mathbf{P}_{op} \cdot \boldsymbol{\sigma}$  depends upon these, as a consequence of the relation:

$$P_{op}^i (\boldsymbol{\sigma} \wedge \mathbf{P}_{op})^j - P_{op}^j (\boldsymbol{\sigma} \wedge \mathbf{P}_{op})^i - P_{op}^2 \varepsilon^{ijk} \sigma_k + \varepsilon^{ijk} P_{k,op} \mathbf{P}_{op} \cdot \boldsymbol{\sigma} = 0. \quad (66)$$

All coefficients of the independent tensors (65) have to be zero. This leads to the solution:

$$f_1(E_{op}) = \frac{\hbar}{2m(E_{op} + mc^2)}, \quad f_2(E_{op}) = 0. \quad (67)$$

If this is substituted into (59) we obtain as the position operator in the P-FW picture:

$$\hat{X}_{op} = \mathbf{R} + \frac{\hbar \boldsymbol{\sigma} \wedge \mathbf{P}_{op}}{2m(E_{op} + mc^2)}. \quad (68)$$

The expression  $\mathbf{X}_{op}$  in the Dirac picture may be found with (56), which implies

$$U_{op}^\dagger = \beta U_{op} \beta \quad (69)$$

and

$$\hat{\boldsymbol{\sigma}}_{op} \equiv U_{op} \boldsymbol{\sigma} U_{op}^\dagger = \boldsymbol{\sigma} + \frac{ic \boldsymbol{\beta} \boldsymbol{\alpha} \wedge \mathbf{P}_{op}}{E_{op}} - \frac{c^2 \mathbf{P}_{op} \wedge (\boldsymbol{\sigma} \wedge \mathbf{P}_{op})}{E_{op}(E_{op} + mc^2)}. \quad (70)$$

Using also (61–63) we get then from (68) the Dirac picture position operator

$$\mathbf{X}_{op} = \mathbf{R} + \frac{i\hbar}{2mc} \boldsymbol{\beta} \left( \boldsymbol{\alpha} - c^2 \frac{\boldsymbol{\alpha} \cdot \mathbf{P}_{op} \mathbf{P}_{op}}{E_{op}^2} \right). \quad (71)$$

In this way the even part of the position operator has been obtained in a unique way by imposing its transformation character. A position operator of this form has been put forward by Pryce<sup>1</sup>.

The part of the spin operator that is even in the P-FW picture may likewise be determined by means of the covariance conditions of the preceding subsection. Indeed from the requirements (37), (39), (41) and (43) for the translation, rotation, spatial inversion and time reversal properties, it follows that the even part of the spin operator, which we shall denote by the symbol  $s_{op}$  in the Dirac picture and by  $\hat{s}_{op}$  in the P-FW picture, has the form<sup>2</sup>

$$\hat{s}_{op} = \{f_1(E_{op}) + \beta f_2(E_{op})\} \boldsymbol{\sigma} + \{f_3(E_{op}) + \beta f_4(E_{op})\} \mathbf{P}_{op} \mathbf{P}_{op} \cdot \boldsymbol{\sigma} \quad (72)$$

with arbitrary real functions  $f_i(E_{op})$  ( $i = 1, \dots, 4$ ). (Indeed  $\boldsymbol{\sigma}$  and  $\mathbf{P}_{op} \mathbf{P}_{op} \cdot \boldsymbol{\sigma}$  are the only axial vectors available. Moreover they have the right time reversal behaviour.) We now substitute this expression into the covariance condition (48), which in the P-FW picture reads

$$[\hat{N}_{op}^i, \hat{s}_{op}^j] = \frac{1}{2} c^{-1} \{ \hat{X}_{op}^i, [H_{op}, \hat{s}_{op}^j] \} - \frac{\hbar}{i} \varepsilon^{ijk} \hat{t}_{k,op}. \quad (73)$$

Then one finds, by noting that the coefficients of the independent (symmetrical) tensors  $P_{op}^i P_{op}^j \mathbf{P}_{op} \cdot \boldsymbol{\sigma}$  and  $\delta^{ij} \mathbf{P}_{op} \cdot \boldsymbol{\sigma}$  must vanish, the form of the functions  $f_i(E_{op})$ . In this way the expression (72) becomes

$$\hat{s}_{op} = (\lambda + \beta \mu) E_{op} \boldsymbol{\sigma} - \frac{\lambda + \beta \mu}{E_{op} + mc^2} c^2 \mathbf{P}_{op} \mathbf{P}_{op} \cdot \boldsymbol{\sigma}, \quad (74)$$

with arbitrary real constants  $\lambda$  and  $\mu$ . Furthermore one obtains from (73) for  $\hat{t}_{op}$ :

$$\hat{t}_{op} = c \beta (\lambda + \beta \mu) \mathbf{P}_{op} \wedge \boldsymbol{\sigma}. \quad (75)$$

The expressions (74) and (75) fulfil the relation (49) (with circumflexes).

From the transformation properties we have found an expression for the spin operator  $\hat{s}_{op}$ , which still contains two arbitrary constants. (The reason for the occurrence of such multiplicative constants is the fact that the covariance requirements (37), (39), (41), (43) and (48) are all linear and homogeneous in  $s_{op}$  and  $t_{op}$ .) To fix the scale we impose a final condition. We require that the sum of the orbital angular momentum  $\mathbf{X}_{op} \wedge \mathbf{P}_{op}$  and the spin angular momentum  $s_{op}$  be equal to the total angular momentum which is the

<sup>1</sup> M. H. L. Pryce, op. cit.

<sup>2</sup> If time reversal is not imposed nothing changes in the expression (72), in contrast with the situation for the position operator.

generator of rotations given by (15):

$$\mathbf{X}_{\text{op}} \wedge \mathbf{P}_{\text{op}} + \mathbf{s}_{\text{op}} = \mathbf{R} \wedge \mathbf{P}_{\text{op}} + \frac{1}{2} \hbar \boldsymbol{\sigma}. \quad (76)$$

Transforming from the Dirac picture to the P-FW picture we find for this condition

$$\hat{\mathbf{X}}_{\text{op}} \wedge \mathbf{P}_{\text{op}} + \hat{\mathbf{s}}_{\text{op}} = \mathbf{R} \wedge \mathbf{P}_{\text{op}} + \frac{1}{2} \hbar \boldsymbol{\sigma}. \quad (77)$$

We could omit some circumflexes, because one has  $\hat{\mathbf{P}}_{\text{op}} = \mathbf{P}_{\text{op}}$  and

$$\hat{\mathbf{R}} \wedge \mathbf{P}_{\text{op}} + \frac{1}{2} \hbar \hat{\boldsymbol{\sigma}}_{\text{op}} = \mathbf{R} \wedge \mathbf{P}_{\text{op}} + \frac{1}{2} \hbar \boldsymbol{\sigma}, \quad (78)$$

as follows from (61–63) and (70). Substituting (68) and (74) into (77) one finds that the constants are  $\lambda = \hbar/2mc^2$  and  $\mu = 0$ , so that finally the even part of the spin operator (74) becomes

$$\hat{\mathbf{s}}_{\text{op}} = \frac{\hbar E_{\text{op}}}{2mc^2} \boldsymbol{\sigma} - \frac{\hbar \mathbf{P}_{\text{op}} \mathbf{P}_{\text{op}} \cdot \boldsymbol{\sigma}}{2m(E_{\text{op}} + mc^2)}, \quad (79)$$

while (75) gets the form:

$$\hat{\mathbf{t}}_{\text{op}} = \frac{\hbar}{2mc} \beta \mathbf{P}_{\text{op}} \wedge \boldsymbol{\sigma}. \quad (80)$$

The spin operator (79) is conserved since it commutes with the Hamiltonian (58).

In the preceding we showed that the covariance properties alone sufficed to fix the position operator  $\hat{\mathbf{X}}_{\text{op}}$  and to find the spin operator  $\hat{\mathbf{s}}_{\text{op}}$  apart from multiplicative constants. It turned out to be possible to choose these constants in such a way that also the total angular momentum condition (77) could be satisfied. (Of course, since in the present case  $\hat{\mathbf{X}}_{\text{op}}$  is completely fixed by the covariance requirements the condition (77) alone would have been sufficient to determine  $\hat{\mathbf{s}}_{\text{op}}$ . However, in view of the fact that such a procedure is not possible in the case with fields – to be considered later – we have not followed this line of reasoning to determine  $\hat{\mathbf{s}}_{\text{op}}$ .)

The operators (79) and (80) are connected by the relation

$$\hat{\mathbf{t}}_{\text{op}} = \frac{\beta c \mathbf{P}_{\text{op}}}{E_{\text{op}}} \wedge \hat{\mathbf{s}}_{\text{op}}. \quad (81)$$

By introducing the velocity operator in the P-FW picture

$$\hat{\mathbf{v}}_{\text{op}} \equiv \frac{i}{\hbar} [\hat{H}_{\text{op}}, \hat{\mathbf{X}}_{\text{op}}] = \frac{\beta c^2 \mathbf{P}_{\text{op}}}{E_{\text{op}}} \quad (82)$$

(where (58) and (68) have been used), one may write the relation (81) also as

$$\hat{\mathbf{t}}_{\text{op}} = c^{-1} \hat{\mathbf{v}}_{\text{op}} \wedge \hat{\mathbf{s}}_{\text{op}}. \quad (83)$$

It is the quantum-mechanical counterpart of the classical relation  $p_\alpha s^{\alpha\beta} = 0$  (IV.67) with  $p^\alpha = mu^\alpha$  (IV.119) for the field-free case.

In the Dirac picture the operators  $\mathbf{s}_{\text{op}}$  and  $\mathbf{t}_{\text{op}}$  follow from (79) and (80):

$$\mathbf{s}_{\text{op}} = \frac{1}{2} \hbar \boldsymbol{\sigma} - \frac{i \hbar \beta \boldsymbol{\alpha} \wedge \mathbf{P}_{\text{op}}}{2mc}, \quad (84)$$

$$\mathbf{t}_{\text{op}} = \frac{\hbar}{2mc} \beta \mathbf{P}_{\text{op}} \wedge \boldsymbol{\sigma}, \quad (85)$$

where we used (70) and:

$$U_{\text{op}} \beta U_{\text{op}}^\dagger = \frac{-c \boldsymbol{\alpha} \cdot \mathbf{P}_{\text{op}} + \beta mc^2}{E_{\text{op}}}, \quad (86)$$

which follows from (2), (58) and (69). The spin operator (84) has been given already by Pryce<sup>1</sup>.

The operators (84) and (85) are the space-space and space-time parts of an antisymmetric tensor

$$s_{\text{op}}^{\mu\nu} = \frac{1}{2} \hbar \sigma^{\mu\nu} + \frac{\hbar}{2mc} (\gamma^\mu P_{\text{op}}^\nu - \gamma^\nu P_{\text{op}}^\mu), \quad (87)$$

where we introduced Dirac matrices  $\gamma^\mu$  ( $\mu = 0, 1, 2, 3$ ) defined as:

$$\gamma^0 \equiv -i\beta, \quad \boldsymbol{\gamma} \equiv -i\beta \boldsymbol{\alpha} \quad (88)$$

and the abbreviation

$$\sigma^{\mu\nu} \equiv -\frac{1}{2} i [\gamma^\mu, \gamma^\nu]. \quad (89)$$

The zero-component  $P_{\text{op}}^0$  of  $P_{\text{op}}^\mu$  is defined to be equal to  $H_{\text{op}}/c$  ( $= \boldsymbol{\alpha} \cdot \mathbf{P}_{\text{op}} + \beta mc$ ). The spin tensor (87) has been found by Fradkin and Good<sup>2</sup> and by Hilgevoord and Wouthuysen<sup>3</sup> starting from a different basis.

The components of the position operator (68) do not commute; in fact one finds the commutation rule

$$[\hat{X}_{\text{op}}^i, \hat{X}_{\text{op}}^j] = i \hbar \epsilon^{ijk} \left( \frac{\hat{s}_{k,\text{op}} c^2}{E_{\text{op}}^2} + \frac{P_{k,\text{op}} \mathbf{P}_{\text{op}} \cdot \hat{\mathbf{s}}_{\text{op}}}{m^2 E_{\text{op}}^2} \right) \quad (90)$$

<sup>1</sup> M. H. L. Pryce, op. cit.

<sup>2</sup> D. M. Fradkin and R. H. Good jr., N. Cim. **22**(1961)643.

<sup>3</sup> J. Hilgevoord and S. A. Wouthuysen, Nucl. Phys. **40**(1963)1.



(it has the same form in the Dirac picture, i.e. without circumflexes). For the components of the spin operator one gets a commutation rule of the form

$$[\hat{s}_{\text{op}}^i, \hat{s}_{\text{op}}^j] = i\hbar \varepsilon^{ijk} \left( \hat{s}_{k,\text{op}} + \frac{P_{k,\text{op}} P_{\text{op}} \cdot \hat{s}_{\text{op}}}{m^2 c^2} \right), \quad (91)$$

(again it has the same form in the Dirac picture).

The requirement of covariant behaviour imposed on the part of the position operator that is even in the P-FW picture has led to non-commuting components. This state of affairs is different from the situation in non-relativistic theory, where one is acquainted with position operators that possess commuting components. (Indeed the right-hand side of (90) is of order  $c^{-2}$ : namely of the order of the square of the Compton wavelength.) Correspondingly the commutation relations for the components of the spin operator do not have the same form as those for the components of the generator  $\mathbf{R} \wedge \mathbf{P}_{\text{op}} + \frac{1}{2}\hbar\boldsymbol{\sigma}$  of spatial rotations<sup>1</sup>.

If in Dirac theory one would impose as a condition the commutation of the Cartesian components of the even part of the position operator one finds, following a similar line of reasoning as above, a position operator which is that of Newton and Wigner<sup>2</sup> (v. appendix):

$$\hat{\mathbf{X}}_{\text{op},\text{NW}} = \mathbf{R}. \quad (92)$$

This operator however does not possess covariant properties as does (68).

It has been tried to reconcile the requirement of covariance and commutation of the components of the position operator. This can only be achieved through an interplay of even and odd parts of the position operator. One obtains in this way the Dirac position and spin operators (v. appendix and <sup>3</sup>). However the even parts alone of these operators violate the covariance condition, and since only these parts occur in the expectation values for positive (or negative) energy solutions the latter will not possess covariant properties. (Still a different position operator may be proposed<sup>4</sup> if apart from the requirement of evenness also the commutivity condition is abandoned.)

<sup>1</sup> M. H. L. Pryce, op. cit., showed that the commutation relations (90) and (91) have classical counterparts in Poisson bracket relations for the components of the centre of energy and the inner angular momentum of a composite particle in classical theory, as discussed in chapter IV.

<sup>2</sup> T. D. Newton and E. P. Wigner, Rev. Mod. Phys. **21**(1949)400.

<sup>3</sup> T. F. Jordan and N. Mukunda, op. cit.; G. Lugarini and M. Pauri, op. cit.

<sup>4</sup> M. Bunge, N. Cim. **1**(1955)977; H. Yamasaki, Progr. Theor. Phys. **31**(1964)322, 324; M. Kolsrud, Phys. Norv. **2**(1967)141, 149.

### 3 The Dirac particle in a field

#### a. Invariance properties

The Dirac Hamiltonian for a particle in an electromagnetic field  $\mathbf{E}(\mathbf{R}, t)$ ,  $\mathbf{B}(\mathbf{R}, t)$ , with potentials  $\varphi(\mathbf{R}, t)$ ,  $\mathbf{A}(\mathbf{R}, t)$ , reads

$$H_{\text{op}} = c\boldsymbol{\alpha}\boldsymbol{\pi}_{\text{op}} + \beta mc^2 + e\varphi + H_{\text{a,op}}, \quad (93)$$

$$H_{\text{a,op}} \equiv \frac{1}{2}(g-2)\mu_{\text{B}}(i\beta\boldsymbol{\alpha}\cdot\mathbf{E} - \beta\boldsymbol{\sigma}\cdot\mathbf{B}), \quad (94)$$

where  $\boldsymbol{\pi}_{\text{op}}$  stands for  $\mathbf{P}_{\text{op}} - (e/c)\mathbf{A}$  and  $\mu_{\text{B}}$  is the Bohr magneton  $e\hbar/2mc$ . The Pauli term  $H_{\text{a,op}}$  represents the coupling of the anomalous magnetic moment with the field.

The Dirac equation (1) with this Hamilton operator is covariant under the transformations of the Poincaré group. One may find (just as in section 2) expressions for the change of the expectation value of an operator under these transformations. In particular we are interested in the change of the expectation value of an operator  $\Omega_{\text{op}}$  that depends on the coordinates  $\mathbf{R}$ , the momentum operator  $\mathbf{P}_{\text{op}} \equiv (\hbar/i)\partial/\partial\mathbf{R}$  and the potentials  $\varphi(\mathbf{R}, t)$  and  $\mathbf{A}(\mathbf{R}, t)$ .

Under an infinitesimal *translation* (6) the expectation value of  $\Omega_{\text{op}}$  changes by an amount which is the expectation value of the operator

$$\delta\Omega_{\text{op}} = \frac{i}{\hbar} \boldsymbol{\varepsilon} \cdot [\mathbf{P}_{\text{op}}, \Omega_{\text{op}}] + \Omega_{\text{op}}(\mathbf{R}, \mathbf{P}_{\text{op}}, \mathbf{A} - \boldsymbol{\varepsilon} \cdot \nabla \mathbf{A}, \varphi - \boldsymbol{\varepsilon} \cdot \nabla \varphi) - \Omega_{\text{op}}(\mathbf{R}, \mathbf{P}_{\text{op}}, \mathbf{A}, \varphi). \quad (95)$$

This may be derived in the same way as (11) is derived in section 2, if one uses the transformation property of  $\varphi$  and  $\mathbf{A}$  under translations:

$$\begin{aligned} \varphi'(\mathbf{R}', t') &= \varphi(\mathbf{R}, t), \\ \mathbf{A}'(\mathbf{R}', t') &= \mathbf{A}(\mathbf{R}, t). \end{aligned} \quad (96)$$

Up to terms with the potentials, but without derivatives of the potentials, (95) simplifies to

$$\delta\Omega_{\text{op}} = \frac{i}{\hbar} \boldsymbol{\varepsilon} \cdot [\mathbf{P}_{\text{op}}, \Omega_{\text{op}}], \quad (97)$$

which is the same expression as (11) for the free particle.

Under an infinitesimal *rotation* (12) the expectation value changes by a term which is the expectation value of the operator

$$\begin{aligned} \delta\Omega_{\text{op}} &= \frac{i}{\hbar} \boldsymbol{\varepsilon} \cdot [\mathbf{R} \wedge \mathbf{P}_{\text{op}} + \frac{1}{2}\hbar\boldsymbol{\sigma}, \Omega_{\text{op}}] \\ &+ \Omega_{\text{op}}(\mathbf{R}, \mathbf{P}_{\text{op}}, \mathbf{A} + \boldsymbol{\varepsilon} \wedge \mathbf{A} - (\boldsymbol{\varepsilon} \wedge \mathbf{R}) \cdot \nabla \mathbf{A}, \varphi - (\boldsymbol{\varepsilon} \wedge \mathbf{R}) \cdot \nabla \varphi) - \Omega_{\text{op}}(\mathbf{R}, \mathbf{P}_{\text{op}}, \mathbf{A}, \varphi), \end{aligned} \quad (98)$$

where we used the transformation property of  $\varphi$  and  $A$  under rotations

$$\begin{aligned}\varphi'(\mathbf{R}', t') &= \varphi(\mathbf{R}, t), \\ A'(\mathbf{R}', t') &= A(\mathbf{R}, t) + \boldsymbol{\varepsilon} \wedge A(\mathbf{R}, t).\end{aligned}\quad (99)$$

Up to terms without derivatives of the potentials the expression (98) is

$$\delta\Omega_{\text{op}} = \frac{i}{\hbar} \boldsymbol{\varepsilon} \cdot [\mathbf{R} \wedge \mathbf{P}_{\text{op}} + \frac{1}{2} \hbar \boldsymbol{\sigma}, \Omega_{\text{op}}] + (\boldsymbol{\varepsilon} \wedge A) \cdot \frac{\partial \Omega_{\text{op}}}{\partial A}. \quad (100)$$

Owing to the presence of the last term, this expression differs from (15) for the field-free case. For a vector operator, which is characterized by (16), the relation (100) becomes:

$$[(\mathbf{R} \wedge \mathbf{P}_{\text{op}} + \frac{1}{2} \hbar \boldsymbol{\sigma})^i, \Omega_{\text{op}}^j] - i \hbar \varepsilon^{imn} A_m \frac{\partial \Omega_{\text{op}}^j}{\partial A^n} = i \hbar \varepsilon^{ijk} \Omega_{k,\text{op}}, \quad (101)$$

which is the generalization of (17) to the case with fields.

In the special case that  $\Omega_{\text{op}}$  is independent of  $\varphi$  and depends on  $A$  only via  $\boldsymbol{\pi}_{\text{op}} \equiv \mathbf{P}_{\text{op}} - (e/c)A$  (i.e.  $\Omega_{\text{op}} = \Omega_{\text{op}}(\mathbf{R}, \boldsymbol{\pi}_{\text{op}})$ ) we have for the last term of (100)

$$- \frac{e}{c} (\boldsymbol{\varepsilon} \wedge A) \cdot \frac{\partial \Omega_{\text{op}}}{\partial \boldsymbol{\pi}_{\text{op}}} = \frac{ie}{\hbar c} [(\boldsymbol{\varepsilon} \wedge A) \cdot \mathbf{R}, \Omega_{\text{op}}]. \quad (102)$$

(The differential quotient stands for the limit  $\lambda \rightarrow 0$  of  $\lambda^{-1} \{ \Omega_{\text{op}}(\mathbf{R}, \boldsymbol{\pi}_{\text{op}} + \boldsymbol{\lambda}) - \Omega_{\text{op}}(\mathbf{R}, \boldsymbol{\pi}_{\text{op}}) \}$ , where  $\boldsymbol{\lambda} = (\lambda, 0, 0)$  and cycl.) Therefore one may write the expression (100) for this special class of operators  $\Omega_{\text{op}}$  as

$$\delta\Omega_{\text{op}} = \frac{i}{\hbar} \boldsymbol{\varepsilon} \cdot [\mathbf{R} \wedge \boldsymbol{\pi}_{\text{op}} + \frac{1}{2} \hbar \boldsymbol{\sigma}, \Omega_{\text{op}}], \quad (103)$$

which has a form analogous to (15), with  $\mathbf{P}_{\text{op}}$  replaced by  $\boldsymbol{\pi}_{\text{op}}$ .

For *spatial inversion* (18) one finds for the expectation value of  $\Omega_{\text{op}}$  in the new frame the expectation value of the operator (cf. (20) for the field-free case):

$$\beta \Omega_{\text{op}}(-\mathbf{R}, -\mathbf{P}_{\text{op}}, -A, \varphi) \beta, \quad (104)$$

where we used the transformation of the potentials:

$$\begin{aligned}\varphi'(\mathbf{R}', t') &= \varphi(\mathbf{R}, t), \\ A'(\mathbf{R}', t') &= -A(\mathbf{R}, t).\end{aligned}\quad (105)$$

Therefore for a polar or axial vector operator one has the relation (cf. (21)):

$$\Omega_{\text{op}}(-\mathbf{R}, -\mathbf{P}_{\text{op}}, -A, \varphi) = \mp \beta \Omega_{\text{op}}(\mathbf{R}, \mathbf{P}_{\text{op}}, A, \varphi) \beta. \quad (106)$$

Under *time reversal* (22) one obtains for the expectation value of  $\Omega_{\text{op}}$  in the new frame the expectation value of the operator (cf. (26) for the field-free case):

$$T \tilde{\Omega}_{\text{op}}(\mathbf{R}, -\mathbf{P}_{\text{op}}, -A, \varphi) T^{-1}, \quad (107)$$

where we used the transformation property of the potentials

$$\begin{aligned}\varphi'(\mathbf{R}', t') &= \varphi(\mathbf{R}, t), \\ A'(\mathbf{R}', t') &= -A(\mathbf{R}, t).\end{aligned}\quad (108)$$

The behaviour of an expectation value under *pure Lorentz transformations* follows from the transformation of the wave function, which is given by an expression as (32) but now with a Hamilton operator  $H_{\text{op}}$  which depends on the potentials  $\varphi(\hat{\mathbf{R}}', t)$  and  $A(\hat{\mathbf{R}}', t)$ . This expression has to be substituted into the transformed expectation value, which reads as (29) but with an operator  $\Omega_{\text{op}}$  which depends also upon the transformed potentials  $\varphi'(\hat{\mathbf{R}}', t')$  and  $A'(\hat{\mathbf{R}}', t')$ . If one uses the transformation formulae for the potentials

$$\begin{aligned}A'(\hat{\mathbf{R}}', t') &= A(\hat{\mathbf{R}}', t) - \boldsymbol{\varepsilon} \varphi(\hat{\mathbf{R}}', t) + ct \boldsymbol{\varepsilon} \cdot \frac{\partial A(\hat{\mathbf{R}}', t)}{\partial \hat{\mathbf{R}}'} + c^{-1} \boldsymbol{\varepsilon} \cdot \hat{\mathbf{R}}' \frac{\partial A(\hat{\mathbf{R}}', t)}{\partial t}, \\ \varphi'(\hat{\mathbf{R}}', t') &= \varphi(\hat{\mathbf{R}}', t) - \boldsymbol{\varepsilon} \cdot A(\hat{\mathbf{R}}', t) + ct \boldsymbol{\varepsilon} \cdot \frac{\partial \varphi(\hat{\mathbf{R}}', t)}{\partial \hat{\mathbf{R}}'} + c^{-1} \boldsymbol{\varepsilon} \cdot \hat{\mathbf{R}}' \frac{\partial \varphi(\hat{\mathbf{R}}', t)}{\partial t},\end{aligned}\quad (109)$$

one finds that the expectation value changes by a quantity which is the expectation value of the operator (cf. (33) for the field-free case):

$$\begin{aligned}\delta\Omega_{\text{op}} &= \frac{i}{\hbar} \boldsymbol{\varepsilon} \cdot [N_{\text{op}} - ct \mathbf{P}_{\text{op}}, \Omega_{\text{op}}] \\ &+ \Omega_{\text{op}} \left( \mathbf{R}, \mathbf{P}_{\text{op}}, A - \boldsymbol{\varepsilon} \varphi + ct \boldsymbol{\varepsilon} \cdot \nabla A + c^{-1} \boldsymbol{\varepsilon} \cdot \mathbf{R} \frac{\partial A}{\partial t}, \right. \\ &\quad \left. \varphi - \boldsymbol{\varepsilon} \cdot A + ct \boldsymbol{\varepsilon} \cdot \nabla \varphi + c^{-1} \boldsymbol{\varepsilon} \cdot \mathbf{R} \frac{\partial \varphi}{\partial t} \right) - \Omega_{\text{op}}(\mathbf{R}, \mathbf{P}_{\text{op}}, A, \varphi),\end{aligned}\quad (110)$$

where  $N_{\text{op}}$  is given by (34) or (35) with (93).

If one confines oneself to terms without the derivatives of the potentials, this expression reduces to

$$\delta\Omega_{\text{op}} = \frac{i}{\hbar} \boldsymbol{\varepsilon} \cdot [N_{\text{op}} - ct \mathbf{P}_{\text{op}}, \Omega_{\text{op}}] - \boldsymbol{\varepsilon} \cdot \frac{\partial \Omega_{\text{op}}}{\partial A} \varphi - \frac{\partial \Omega_{\text{op}}}{\partial \varphi} \boldsymbol{\varepsilon} \cdot A. \quad (111)$$

In particular if the operator  $\Omega_{\text{op}}$  is independent of  $\varphi$  and depends on  $A$  only

through  $\pi_{\text{op}} \equiv \mathbf{P}_{\text{op}} - (e/c)\mathbf{A}$ , the last two terms become

$$\frac{e}{c} \boldsymbol{\varepsilon} \cdot \frac{\partial \Omega_{\text{op}}}{\partial \pi_{\text{op}}} \varphi = - \frac{ie}{\hbar c} [\boldsymbol{\varepsilon} \cdot \mathbf{R} \varphi, \Omega_{\text{op}}], \quad (112)$$

so that (111) gets the form:

$$\delta \Omega_{\text{op}} = \frac{i}{\hbar} \boldsymbol{\varepsilon} \cdot [N_{\text{op}}^{(\varphi)} - ct \mathbf{P}_{\text{op}}, \Omega_{\text{op}}], \quad (113)$$

where we used the abbreviation

$$N_{\text{op}}^{(\varphi)} \equiv N_{\text{op}} - (e/c)\mathbf{R}\varphi = \frac{1}{2}c^{-1}\{\mathbf{R}, H_{\text{op}} - e\varphi\}. \quad (114)$$

In the last member the definition (34) or (35) has been used.

#### b. Covariance requirements on the position and spin operators for a particle in a field

The position and spin operators for a free Dirac particle have been found in section 2. If the particle moves in an electromagnetic field the problem of the derivation of the position and spin operators should be reconsidered from the beginning. The expression for these operators should reduce to those of the field-free case if the fields are switched off. In the presence of fields the position and spin operators will contain additional terms with the potentials and their derivatives with respect to time and space coordinates. In the following we shall be interested only in those additional terms which contain the potentials, not their derivatives. These additional terms will be determined by imposing a number of conditions just as in the field-free case. In this section we shall be concerned with the requirements of covariance with respect to the Poincaré group.

As *translation* properties we impose again (36–37) on the position and spin operator. As *rotation* properties we require that both the position and spin operator be vector operators, so that we have, in view of (101),

$$[(\mathbf{R} \wedge \mathbf{P}_{\text{op}} + \frac{1}{2}\hbar\boldsymbol{\sigma})^i, X_{\text{op}}^j] - i\hbar\varepsilon^{imn}A_m \frac{\partial X_{\text{op}}^j}{\partial A^n} = i\hbar\varepsilon^{ijk}X_{k,\text{op}}, \quad (115)$$

$$[(\mathbf{R} \wedge \mathbf{P}_{\text{op}} + \frac{1}{2}\hbar\boldsymbol{\sigma})^i, s_{\text{op}}^j] - i\hbar\varepsilon^{imn}A_m \frac{\partial s_{\text{op}}^j}{\partial A^n} = i\hbar\varepsilon^{ijk}s_{k,\text{op}}. \quad (116)$$

As to the properties under *spatial inversion*, we require that the position operator be a polar vector and the spin operator an axial vector. We have

thus from (106)

$$\mathbf{X}_{\text{op}}(-\mathbf{R}, -\mathbf{P}_{\text{op}}, -\mathbf{A}, \varphi) = -\beta\mathbf{X}_{\text{op}}(\mathbf{R}, \mathbf{P}_{\text{op}}, \mathbf{A}, \varphi)\beta, \quad (117)$$

$$s_{\text{op}}(-\mathbf{R}, -\mathbf{P}_{\text{op}}, -\mathbf{A}, \varphi) = \beta s_{\text{op}}(\mathbf{R}, \mathbf{P}_{\text{op}}, \mathbf{A}, \varphi)\beta. \quad (118)$$

Under *time reversal* the expectation value of the position operator should remain invariant, while the spin operator must change sign, so that one must have in view of (107)

$$\mathbf{X}_{\text{op}}(\mathbf{R}, -\mathbf{P}_{\text{op}}, -\mathbf{A}, \varphi) = T\tilde{\mathbf{X}}_{\text{op}}(\mathbf{R}, \mathbf{P}_{\text{op}}, \mathbf{A}, \varphi)T^{-1}, \quad (119)$$

$$s_{\text{op}}(\mathbf{R}, -\mathbf{P}_{\text{op}}, -\mathbf{A}, \varphi) = -T\tilde{s}_{\text{op}}(\mathbf{R}, \mathbf{P}_{\text{op}}, \mathbf{A}, \varphi)T^{-1}. \quad (120)$$

For the transformation property of the position operator under a *pure Lorentz transformation* we postulate, just as in the field-free case (cf. (44)), that

$$\delta \mathbf{X}_{\text{op}} = -\varepsilon ct + \frac{i}{2\hbar c} \{\boldsymbol{\varepsilon} \cdot \mathbf{X}_{\text{op}}, [H_{\text{op}}, \mathbf{X}_{\text{op}}]\}, \quad (121)$$

but where now the Hamilton operator  $H_{\text{op}}$  stands for the expression (93). With (111) for  $\boldsymbol{\Omega}_{\text{op}} = \mathbf{X}_{\text{op}}$  and (36) we find from (121)

$$[N_{\text{op}}^i, X_{\text{op}}^j] - \frac{\hbar}{i} \left( \frac{\partial X_{\text{op}}^j}{\partial A_i} \varphi + \frac{\partial X_{\text{op}}^j}{\partial \varphi} A^i \right) = \frac{1}{2}c^{-1}\{X_{\text{op}}^i, [H_{\text{op}}, X_{\text{op}}^j]\}. \quad (122)$$

For the transformation property of the spin operator under a *pure Lorentz transformation* we also postulate an equation of the same form as in the field-free case i.e. (46–47), but with  $H_{\text{op}}$  (93) inserted. With (37) and (111) for  $\boldsymbol{\Omega}_{\text{op}} = s_{\text{op}}$  we find from (46–47):

$$[N_{\text{op}}^i, s_{\text{op}}^j] - \frac{\hbar}{i} \left( \frac{\partial s_{\text{op}}^j}{\partial A_i} \varphi + \frac{\partial s_{\text{op}}^j}{\partial \varphi} A^i \right) = \frac{1}{2}c^{-1}\{X_{\text{op}}^i, [H_{\text{op}}, s_{\text{op}}^j]\} - \frac{\hbar}{i} \varepsilon^{ijk}t_{k,\text{op}}, \quad (123)$$

with the three-vector operator  $t_{\text{op}}$  such that

$$[N_{\text{op}}^i, t_{\text{op}}^j] - \frac{\hbar}{i} \left( \frac{\partial t_{\text{op}}^j}{\partial A_i} \varphi + \frac{\partial t_{\text{op}}^j}{\partial \varphi} A^i \right) = \frac{1}{2}c^{-1}\{X_{\text{op}}^i, [H_{\text{op}}, t_{\text{op}}^j]\} + \frac{\hbar}{i} \varepsilon^{ijk}s_{k,\text{op}}. \quad (124)$$

In the following we shall find the position and spin operators up to terms in the potentials by using the covariance requirements given above. We first have to transform the Hamilton operator for a Dirac particle in a field. It will be convenient to use Weyl transforms in the course of the reasoning. For that reason a short digression on Weyl transforms, in particular their generalization to operators pertaining to particles with internal degrees of freedom, will now be given.

c. *Weyl transforms for particles with spin*

In chapter VI the theory of Weyl transforms of operators for point particles was considered. If the particles have structure, this method has to be generalized somewhat. (See also the appendix of chapter VI for details.) Indeed to every eigenvalue  $\mathbf{p}$  and  $\mathbf{q}$  of the momentum and coordinate operators  $\mathbf{P}$  and  $\mathbf{Q}$ <sup>1</sup> now correspond several eigenstates, which will be labelled by an extra index:

$$\mathbf{P}|\mathbf{p}, \kappa\rangle = \mathbf{p}|\mathbf{p}, \kappa\rangle, \quad \mathbf{Q}|\mathbf{q}, \kappa\rangle = \mathbf{q}|\mathbf{q}, \kappa\rangle. \quad (125)$$

In Dirac theory  $\kappa$  assumes the values 1, 2, 3 or 4. From this basis we construct the operator

$$\Omega_{\kappa\lambda} = \int d\mathbf{p}|\mathbf{p}, \kappa\rangle\langle\mathbf{p}, \lambda| = \int d\mathbf{q}|\mathbf{q}, \kappa\rangle\langle\mathbf{q}, \lambda|, \quad (126)$$

which transforms the subspace of Hilbert space labelled by  $\lambda$  into that labelled by  $\kappa$ .

The Weyl transform of an operator  $A$  may be defined in a way which is analogous to that of the theory of point particles. One gets (cf. (VI.14) and (VI.26)):

$$\begin{aligned} a_{\kappa\lambda}(\mathbf{p}, \mathbf{q}) &= \int d\mathbf{u} e^{(i\hbar)\mathbf{q}\cdot\mathbf{u}} \langle\mathbf{p} + \frac{1}{2}\mathbf{u}, \kappa|A|\mathbf{p} - \frac{1}{2}\mathbf{u}, \lambda\rangle \\ &= \int d\mathbf{v} e^{(i\hbar)\mathbf{p}\cdot\mathbf{v}} \langle\mathbf{q} - \frac{1}{2}\mathbf{v}, \kappa|A|\mathbf{q} + \frac{1}{2}\mathbf{v}, \lambda\rangle. \end{aligned} \quad (127)$$

The Weyl transform thus depends on a pair of labels  $\kappa\lambda$ . From the Weyl transform one may recover the operator (cf. (VI.13)):

$$A = \hbar^{-3} \sum_{\kappa, \lambda} \int d\mathbf{p} d\mathbf{q} a_{\kappa\lambda}(\mathbf{p}, \mathbf{q}) \Delta_{\kappa\lambda}(\mathbf{p}, \mathbf{q}). \quad (128)$$

Here the operator  $\Delta_{\kappa\lambda}(\mathbf{p}, \mathbf{q})$  is given by

$$\Delta_{\kappa\lambda}(\mathbf{p}, \mathbf{q}) = \Delta(\mathbf{p}, \mathbf{q}) \Omega_{\kappa\lambda} \quad (129)$$

with the two operators  $\Delta(\mathbf{p}, \mathbf{q})$  (VI.15) and  $\Omega_{\kappa\lambda}$  (126).

In the special case that the operator  $A$  does not connect the different parts of Hilbert space labelled by  $\kappa$  and acts moreover in each subspace in the same way, one finds from (127) that its Weyl transform has the form

$$a_{\kappa\lambda}(\mathbf{p}, \mathbf{q}) = \delta_{\kappa\lambda} a(\mathbf{p}, \mathbf{q}), \quad (130)$$

where  $a(\mathbf{p}, \mathbf{q})$  is independent of  $\kappa$  and  $\lambda$ .

<sup>1</sup> In this subsection we use capitals for operators and lower case symbols for  $c$ -numbers.

If the operator  $A$  is independent of the coordinate and momentum operators (as for instance the Dirac matrices) its Weyl transform (127) is independent of  $\mathbf{p}$  and  $\mathbf{q}$ :

$$a_{\kappa\lambda}(\mathbf{p}, \mathbf{q}) = a_{\kappa\lambda}. \quad (131)$$

For the Weyl transform of a product of operators one obtains (cf. (VI.42))

$$AB \rightleftharpoons \exp\left\{\frac{i\hbar}{2}\left(\frac{\partial^{(a)}}{\partial\mathbf{q}} \cdot \frac{\partial^{(b)}}{\partial\mathbf{p}} - \frac{\partial^{(a)}}{\partial\mathbf{p}} \cdot \frac{\partial^{(b)}}{\partial\mathbf{q}}\right)\right\} \sum_{\mu} a_{\kappa\mu}(\mathbf{p}, \mathbf{q}) b_{\mu\lambda}(\mathbf{p}, \mathbf{q}). \quad (132)$$

This expression permits to find the Weyl transforms of the commutator and anticommutator of two operators as well (see chapter VI, formulae (A160–161)).

d. *Transformation of the Hamilton operator*

The Hamiltonian (93) will be put to even form by three successive transformations. First a transformation will be performed<sup>1</sup> with the operator

$$S_{1,\text{op}} \rightleftharpoons \frac{E_{\pi} + mc^2 + c\beta\boldsymbol{\alpha}\cdot\boldsymbol{\pi}}{\{2E_{\pi}(E_{\pi} + mc^2)\}^{\frac{1}{2}}}, \quad (133)$$

where we used the abbreviation

$$E_{\pi} \equiv (c^2\boldsymbol{\pi}^2 + m^2c^4)^{\frac{1}{2}}, \quad (134)$$

with  $\boldsymbol{\pi} \equiv \mathbf{P} - (e/c)\mathbf{A}$ . At the right-hand side of (133) the Weyl transform has been written. If  $e = 0$ , the operator  $S_{1,\text{op}}$  reduces to  $U_{\text{op}}$  (56) of which the Weyl transform will be denoted by  $U$ . If only terms linear in  $e$  and without second and higher derivatives of the potentials are taken into account we find

$$\begin{aligned} S_{1,\text{op}} H_{\text{op}} S_{1,\text{op}}^{\dagger} &\rightleftharpoons S_1 H S_1^{\dagger} + \frac{ie\hbar}{2c} \varepsilon_{ijk} \frac{\partial U}{\partial P_i} \frac{\partial H}{\partial P_j} U^{\dagger} B^k + \frac{ie\hbar}{2c} \varepsilon_{ijk} U \frac{\partial H}{\partial P_i} \frac{\partial U^{\dagger}}{\partial P_j} B^k \\ &+ \frac{ie\hbar}{2c} \varepsilon_{ijk} \frac{\partial U}{\partial P_i} H \frac{\partial U^{\dagger}}{\partial P_j} B^k - \frac{ie\hbar}{2} \frac{\partial U}{\partial P_i} \frac{\partial \varphi}{\partial R^i} U^{\dagger} + \frac{ie\hbar}{2} U \frac{\partial \varphi}{\partial R_i} \frac{\partial U^{\dagger}}{\partial P^i}, \end{aligned} \quad (135)$$

since the Weyl transform of  $S_{1,\text{op}}$  depends on  $\mathbf{P}$  and  $\mathbf{R}$  only through  $\boldsymbol{\pi}$ . Here the same symbols are used for operators (l.h.s.) and their Weyl transforms (r.h.s.). The operator  $S_{1,\text{op}}$  is not unitary since

$$S_{1,\text{op}} S_{1,\text{op}}^{\dagger} \rightleftharpoons 1 + \frac{ie\hbar}{2c} \varepsilon_{ijk} \frac{\partial U}{\partial P_i} \frac{\partial U^{\dagger}}{\partial P_j} B^k. \quad (136)$$

<sup>1</sup> E. I. Blount, Phys. Rev. **126**(1962)1636, **128**(1962)2454.

However the product  $U_{1,\text{op}} = S_{2,\text{op}}S_{1,\text{op}}$  is unitary (up to terms linear in  $e$  and without second and higher derivatives of the potentials), if  $S_{2,\text{op}}$  is chosen such that

$$S_{2,\text{op}} \rightleftharpoons 1 - \frac{ie\hbar}{4c} \varepsilon_{ijk} \frac{\partial U}{\partial P_i} \frac{\partial U^\dagger}{\partial P_j} B^k. \quad (137)$$

The transformed Hamiltonian becomes

$$\begin{aligned} U_{1,\text{op}} H_{\text{op}} U_{1,\text{op}}^\dagger &\rightleftharpoons S_1 H S_1^\dagger + \frac{ie\hbar}{2c} \varepsilon_{ijk} \frac{\partial U}{\partial P_i} \frac{\partial H}{\partial P_j} U^\dagger B^k + \frac{ie\hbar}{2c} \varepsilon_{ijk} U \frac{\partial H}{\partial P_i} \frac{\partial U^\dagger}{\partial P_j} B^k \\ &+ \frac{ie\hbar}{2c} \varepsilon_{ijk} \frac{\partial U}{\partial P_i} H \frac{\partial U^\dagger}{\partial P_j} B^k - \frac{ie\hbar}{2} \frac{\partial U}{\partial P_i} \frac{\partial \varphi}{\partial R^i} U^\dagger + \frac{ie\hbar}{2} U \frac{\partial \varphi}{\partial R_i} \frac{\partial U^\dagger}{\partial P^i} \\ &- \frac{ie\hbar}{4c} \varepsilon_{ijk} \frac{\partial U}{\partial P_i} \frac{\partial U^\dagger}{\partial P_j} B^k \beta E - \frac{ie\hbar}{4c} \beta E \varepsilon_{ijk} \frac{\partial U}{\partial P_i} \frac{\partial U^\dagger}{\partial P_j} B^k. \end{aligned} \quad (138)$$

We now introduce the abbreviation  $\xi$  (62) and employ the identity

$$U \frac{\partial H}{\partial \mathbf{P}} U^\dagger = \frac{\partial}{\partial \mathbf{P}} (U H U^\dagger) - \frac{\partial U}{\partial \mathbf{P}} H U^\dagger - U H \frac{\partial U^\dagger}{\partial \mathbf{P}} = \beta \frac{c^2 \mathbf{P}}{E} + \frac{2i}{\hbar} E \beta \xi_o, \quad (139)$$

where  $o$  (and  $e$ ) denote odd (and even) parts. In the last member we used the Weyl transform of (58) and (62). Then (138) becomes

$$\begin{aligned} U_{1,\text{op}} H_{\text{op}} U_{1,\text{op}}^\dagger &\rightleftharpoons \beta E_\pi + e\varphi - \frac{ieE}{2\hbar c} \varepsilon_{ijk} \{\xi^i, \beta \xi_o^j\} B^k \\ &- \frac{ec}{E} \beta \xi_c \cdot (\mathbf{P} \wedge \mathbf{B}) + e\xi \cdot \frac{\hat{c}\varphi}{\partial \mathbf{R}} + \frac{1}{2}(g-2)\mu_B U(i\beta \boldsymbol{\alpha} \cdot \mathbf{E} - \beta \boldsymbol{\sigma} \cdot \mathbf{B}) U^\dagger. \end{aligned} \quad (140)$$

Since the time derivative of the transformed wave function is determined by  $\{U_1 H U_1^\dagger - (\hbar/i)(\partial U_1/\partial t) U_1^\dagger\}_{\text{op}}$  we also need  $\partial U_{1,\text{op}}/\partial t$  of which the Weyl transform is  $-(e/c)(\partial U/\partial \mathbf{P}) \cdot (\partial \mathbf{A}/\partial t)$  (up to terms linear in  $e$  and without second derivatives of the potentials). We obtain thus

$$\begin{aligned} U_{1,\text{op}} H_{\text{op}} U_{1,\text{op}}^\dagger - (\hbar/i)(\partial U_{1,\text{op}}/\partial t) U_{1,\text{op}}^\dagger &\rightleftharpoons \beta E_\pi + e\varphi - \frac{ieE}{2\hbar c} \varepsilon_{ijk} \{\xi^i, \beta \xi_o^j\} B^k \\ &- \frac{ec}{E} \beta \xi_c \cdot (\mathbf{P} \wedge \mathbf{B}) - e\xi \cdot \mathbf{E} + \frac{1}{2}(g-2)\mu_B U(i\beta \boldsymbol{\alpha} \cdot \mathbf{E} - \beta \boldsymbol{\sigma} \cdot \mathbf{B}) U^\dagger. \end{aligned} \quad (141)$$

Here the odd terms which depend on the fields may be transformed away by means of a final unitary (up to terms linear in  $e$  and without second and higher derivatives of the potentials) transformation

$$\begin{aligned} U_{2,\text{op}} &\rightleftharpoons 1 - \frac{ie}{4\hbar c} \varepsilon_{ijk} \{\xi^i, \xi_o^j\} B^k \\ &- \frac{e}{2E} \beta \xi_o \cdot \mathbf{E} + \frac{(g-2)\mu_B}{4E} \beta \{U(i\beta \boldsymbol{\alpha} \cdot \mathbf{E} - \beta \boldsymbol{\sigma} \cdot \mathbf{B}) U^\dagger\}_o. \end{aligned} \quad (142)$$

The explicit transformed Hamiltonian is obtained if we substitute the expressions (63). The result is – up to terms linear in  $e$  and without second and higher derivatives of the potentials –

$$\begin{aligned} \hat{H}_{\text{op}} &\equiv U_{2,\text{op}} U_{1,\text{op}} H_{\text{op}} U_{1,\text{op}}^\dagger U_{2,\text{op}}^\dagger - \frac{\hbar}{i} \frac{\partial (U_{2,\text{op}} U_{1,\text{op}})}{\partial t} U_{1,\text{op}}^\dagger U_{2,\text{op}}^\dagger \\ &\rightleftharpoons \beta E_\pi + e\varphi - \mu_B \frac{mc^2}{E} \beta \boldsymbol{\sigma} \cdot \mathbf{B} - \mu_B \frac{mc^3}{E(E+mc^2)} (\mathbf{P} \wedge \boldsymbol{\sigma}) \cdot \mathbf{E} \\ &- \frac{1}{2}(g-2)\mu_B \left\{ \beta \boldsymbol{\sigma} \cdot \mathbf{B} - \frac{\beta c^2 \mathbf{P} \cdot \boldsymbol{\sigma} \mathbf{P} \cdot \mathbf{B}}{E(E+mc^2)} + \frac{c(\mathbf{P} \wedge \boldsymbol{\sigma}) \cdot \mathbf{E}}{E} \right\}, \end{aligned} \quad (143)$$

which is the relativistic generalization of the expression derived by Foldy–Wouthuysen<sup>1</sup>. Apart from the anomalous terms it has been found by Blount<sup>2</sup>. We shall call it the Hamiltonian in the Blount picture.

### *e. Covariant position and spin operators*

In order to obtain the equation of motion up to second order derivatives of the potentials an expression for the position operator including terms with the potentials will be needed. Since the Hamiltonian (143) in the Blount picture is even only the even part  $\hat{X}_{\text{op}}$  of the position operator in the Blount picture is relevant. This part is fixed by a set of conditions. In the first place the expression  $\hat{X}_{\text{op}}$  in the Blount picture should reduce to the form (68) for the field-free case. If furthermore the transformation properties of  $X_{\text{op}}$  under translations (36), rotations (115), spatial inversion (117), time reversal (119) with  $T = \sigma_2$  in the Pauli representation and pure Lorentz transformations (122) are taken into account it follows after a straightforward but rather long calculation, that in the Blount picture  $\hat{X}_{\text{op}}$  has the form

$$\begin{aligned} \hat{X}_{\text{op}} &\rightleftharpoons \mathbf{R} + \frac{\hbar \boldsymbol{\sigma} \wedge \boldsymbol{\pi}}{2m(E_\pi + mc^2)} \\ &+ (a_1 + \beta a_2) \left\{ \frac{c}{E} \mathbf{P} \wedge \boldsymbol{\sigma} \mathbf{P} \cdot \mathbf{A} + \frac{m^2 c^3}{E} \mathbf{A} \wedge \boldsymbol{\sigma} - \frac{mc^3 \mathbf{P} \wedge \mathbf{A} \mathbf{P} \cdot \boldsymbol{\sigma}}{E(E+mc^2)} - \beta \mathbf{P} \wedge \boldsymbol{\sigma} \varphi \right\}, \end{aligned} \quad (144)$$

<sup>1</sup> L. L. Foldy and S. A. Wouthuysen, op. cit.

<sup>2</sup> E. I. Blount, op. cit.

where  $a_1$  and  $a_2$  are real arbitrary constants. The velocity operator (up to terms with the potentials) corresponding to this position operator follows with (143):

$$\hat{v}_{\text{op}} \equiv \frac{i}{\hbar} [\hat{H}_{\text{op}}, \hat{X}_{\text{op}}] \rightleftharpoons \beta c^2 \pi / E_\pi \equiv \hat{v}. \quad (145)$$

In an analogous way the even part  $\hat{s}_{\text{op}}$  of the spin operator in the Blount picture up to terms with the potentials (which should reduce to (79) in the field-free case) is found by fixing its transformation properties under translations (37), rotations (116), spatial inversion (118), time reversal (120) with  $T = \sigma_2$  and pure Lorentz transformations (123–124). We obtain

$$\begin{aligned} \hat{s}_{\text{op}} \rightleftharpoons & \frac{\hbar E_\pi}{2mc^2} \boldsymbol{\sigma} - \frac{\hbar \pi \boldsymbol{\pi} \cdot \boldsymbol{\sigma}}{2m(E_\pi + mc^2)} + (b_1 + \beta b_2) \left( \boldsymbol{A} \boldsymbol{P} \cdot \boldsymbol{\sigma} - mc \beta \boldsymbol{\sigma} \boldsymbol{\varphi} - \frac{\beta c \boldsymbol{P} \boldsymbol{P} \cdot \boldsymbol{\sigma} \boldsymbol{\varphi}}{E + mc^2} \right) \\ & + (b_3 + \beta b_4) \left( \frac{c \boldsymbol{P} \boldsymbol{P} \cdot \boldsymbol{A} \boldsymbol{P} \cdot \boldsymbol{\sigma}}{E + mc^2} - c^{-1} E \boldsymbol{\sigma} \boldsymbol{P} \cdot \boldsymbol{A} - \frac{\beta E \boldsymbol{P} \boldsymbol{P} \cdot \boldsymbol{\sigma} \boldsymbol{\varphi}}{E + mc^2} + c^{-2} \beta E^2 \boldsymbol{\sigma} \boldsymbol{\varphi} \right). \end{aligned} \quad (146)$$

The operator  $\hat{t}_{\text{op}}$ , which is connected with  $s_{\text{op}}$  according to (123–124), is in the Blount picture:

$$\begin{aligned} \hat{t}_{\text{op}} \rightleftharpoons & \frac{\hbar \beta \boldsymbol{\pi} \wedge \boldsymbol{\sigma}}{2mc} + (b_1 + \beta b_2) \left( mc \beta \boldsymbol{\sigma} \wedge \boldsymbol{A} + \frac{c \beta \boldsymbol{P} \wedge \boldsymbol{A} \boldsymbol{P} \cdot \boldsymbol{\sigma}}{E + mc^2} \right) \\ & + (b_3 + \beta b_4) (\beta \boldsymbol{\sigma} \wedge \boldsymbol{P} \boldsymbol{P} \cdot \boldsymbol{A} + c^{-1} E \boldsymbol{\varphi} \boldsymbol{P} \wedge \boldsymbol{\sigma}). \end{aligned} \quad (147)$$

A further constraint on the spin operator follows from the orthogonality condition

$$c^{-1} \hat{v}_{\text{op}} \wedge \hat{s}_{\text{op}} = \hat{t}_{\text{op}}, \quad (148)$$

which is the quantum-mechanical counterpart (up to terms with the potentials) of the classical condition  $p_\alpha s^{\alpha\beta} = 0$  (IV.67) with (IV.152). It is satisfied if  $b_1$  and  $b_2$  vanish.

The position operator and the spin operator are not independent of each other. As a generalization of the field-free case we shall require that the sum of the orbital angular momentum  $X_{\text{op}} \wedge \pi_{\text{op}}$  and the spin  $s_{\text{op}}$  be equal to the operator  $\boldsymbol{R} \wedge \boldsymbol{\pi}_{\text{op}} + \frac{1}{2} \hbar \boldsymbol{\sigma}$  in the Dirac picture. As shown in (103) this quantity is the generator of rotations for a special class of operators. The requirement reads written in the Blount picture

$$\hat{X}_{\text{op}} \wedge \boldsymbol{\pi}_{\text{op}} + \hat{s}_{\text{op}} = \boldsymbol{R} \wedge \boldsymbol{\pi}_{\text{op}} + \frac{1}{2} \hbar \boldsymbol{\sigma}. \quad (149)$$

If (144) and (146) are inserted we get the result that the remaining constants

$a_1, a_2, b_3$  and  $b_4$  vanish as well, so that finally we obtain in the Blount picture

$$\hat{X}_{\text{op}} \rightleftharpoons \boldsymbol{R} + \frac{\hbar \boldsymbol{\sigma} \wedge \boldsymbol{\pi}}{2m(E_\pi + mc^2)}, \quad (150)$$

$$\hat{s}_{\text{op}} \rightleftharpoons \frac{\hbar E_\pi}{2mc^2} \boldsymbol{\sigma} - \frac{\hbar \pi \boldsymbol{\pi} \cdot \boldsymbol{\sigma}}{2m(E_\pi + mc^2)} \quad (151)$$

and in the Dirac picture

$$X_{\text{op}} \rightleftharpoons \boldsymbol{R} + \frac{i\hbar}{2mc} \beta \left( \boldsymbol{\alpha} - c^2 \frac{\boldsymbol{\alpha} \cdot \boldsymbol{\pi} \boldsymbol{\pi}}{E_\pi} \right), \quad (152)$$

$$s_{\text{op}} \rightleftharpoons \frac{1}{2} \hbar \boldsymbol{\sigma} - \frac{i\hbar \beta \boldsymbol{\alpha} \wedge \boldsymbol{\pi}}{2mc} \quad (153)$$

as position and spin operators.

With the help of these final results for the position and spin operators up to terms with the potentials we shall derive equations of motion and spin.

#### f. Equations of motion and of spin

The equation of motion for the Dirac particle is obtained by taking twice the total time derivative (with the use of the Hamiltonian (143)) of the position operator in the Blount picture. In the first place we have to evaluate the velocity operator. The Weyl transform of the commutator  $[\hat{H}_{\text{op}}, \hat{X}_{\text{op}}]$  can be expressed in terms of the Weyl transforms of  $\hat{H}_{\text{op}}$  and  $\hat{X}_{\text{op}}$  with the use of (132). Up to terms linear in  $e$  and without field derivatives one obtains for the velocity operator (cf. (145)):

$$\begin{aligned} \hat{v}_{\text{op}} \equiv \frac{d\hat{X}_{\text{op}}}{dt} & \equiv \frac{i}{\hbar} [\hat{H}_{\text{op}}, \hat{X}_{\text{op}}] + \frac{\partial \hat{X}_{\text{op}}}{\partial t} \\ & \rightleftharpoons \frac{\beta \boldsymbol{\pi} c^2}{E_\pi} - \frac{e\hbar c \beta \boldsymbol{\sigma} \boldsymbol{P} \cdot \boldsymbol{B}}{2mE(E + mc^2)} + \frac{e\hbar c \beta \boldsymbol{P} \boldsymbol{\sigma} \cdot \boldsymbol{B} (E^2 + E mc^2 + m^2 c^4)}{2mE^3 (E + mc^2)} \\ & + \frac{e\hbar c^2 \boldsymbol{P} (\boldsymbol{P} \wedge \boldsymbol{\sigma}) \cdot \boldsymbol{E}}{2mE^3} + \frac{1}{2} (g - 2) \mu_B \left\{ \frac{\beta \boldsymbol{P} \cdot \boldsymbol{\sigma} \boldsymbol{B}}{mE} - \frac{\beta c^2 \boldsymbol{P} \boldsymbol{P} \cdot \boldsymbol{\sigma} \boldsymbol{P} \cdot \boldsymbol{B}}{mE^3} \right. \\ & \left. + \frac{c \boldsymbol{E} \wedge \boldsymbol{\sigma}}{E} + \frac{c^3 \boldsymbol{P} (\boldsymbol{P} \wedge \boldsymbol{\sigma}) \cdot \boldsymbol{E}}{E^3} - \frac{c \boldsymbol{P} \cdot \boldsymbol{\sigma} \boldsymbol{P} \wedge \boldsymbol{E}}{mE(E + mc^2)} \right\}. \end{aligned} \quad (154)$$

Likewise the acceleration operator may be calculated up to terms linear in  $e$  and with first derivatives of the field

$$\begin{aligned}
\frac{d^2\hat{X}_{\text{op}}}{dt^2} &\equiv \frac{d\hat{v}_{\text{op}}}{dt} \equiv \frac{i}{\hbar} [\hat{H}_{\text{op}}, \hat{v}_{\text{op}}] + \frac{\partial\hat{v}_{\text{op}}}{\partial t} \rightleftharpoons \frac{c^2}{E} \left( \mathbf{U} - \frac{c^2\mathbf{P}\mathbf{P}}{E^2} \right) \\
&\cdot \left[ e\beta\mathbf{E} + \frac{ec}{E} \mathbf{P} \wedge \mathbf{B} + \mu_{\text{B}} \left\{ \frac{mc^2}{E} (\nabla\mathbf{B}) \cdot \boldsymbol{\sigma} + \frac{\beta mc^3}{E(E+mc^2)} (\nabla\mathbf{E}) \cdot (\mathbf{P} \wedge \boldsymbol{\sigma}) \right\} \right. \\
&+ \mu_{\text{B}} \left( \frac{\partial}{\partial t} + \frac{\beta c^2 \mathbf{P} \cdot \nabla}{E} \right) \left\{ \frac{\mathbf{P}(\mathbf{P} \wedge \boldsymbol{\sigma}) \cdot \mathbf{E}}{m^2 c^3} - \frac{\beta \boldsymbol{\sigma} \mathbf{P} \cdot \mathbf{B}}{E+mc^2} + \beta \frac{\mathbf{P} \boldsymbol{\sigma} \cdot \mathbf{B} (E^2 + E mc^2 + m^2 c^4)}{m^2 c^4 (E+mc^2)} \right. \\
&- \left. \left. \frac{\beta \mathbf{P} \mathbf{P} \cdot \boldsymbol{\sigma} \mathbf{P} \cdot \mathbf{B}}{m^2 c^2 (E+mc^2)} \right\} + \frac{1}{2}(g-2)\mu_{\text{B}} \left\{ (\nabla\mathbf{B}) \cdot \boldsymbol{\sigma} - \frac{c^2 (\nabla\mathbf{B}) \cdot \mathbf{P} \mathbf{P} \cdot \boldsymbol{\sigma}}{E(E+mc^2)} - \beta \frac{c (\nabla\mathbf{E}) \cdot (\boldsymbol{\sigma} \wedge \mathbf{P})}{E} \right\} \right. \\
&\left. + \frac{1}{2}(g-2)\mu_{\text{B}} \left( \frac{\partial}{\partial t} + \frac{\beta c^2 \mathbf{P} \cdot \nabla}{E} \right) \left\{ c^{-1} \mathbf{E} \wedge \boldsymbol{\sigma} + \frac{\beta \boldsymbol{\sigma} \cdot \mathbf{P} \mathbf{B}}{mc^2} - \frac{\mathbf{P} \cdot \boldsymbol{\sigma} \mathbf{P} \wedge \mathbf{E}}{mc(E+mc^2)} \right\} \right]. \quad (155)
\end{aligned}$$

(The time and space derivations act only on the fields.) The first terms at the right-hand side contain the fields  $\mathbf{E}(\mathbf{R}, t)$  and  $\mathbf{B}(\mathbf{R}, t)$  as functions of the space coordinate in the Blount picture. Since the position of the particle is given by  $\hat{X}$  (150), we now wish to introduce the fields as functions of  $\hat{X}$ . Then we obtain for the first two terms on the right-hand side of (155) up to terms linear in  $e$  and with first derivatives of the fields

$$e\beta\mathbf{E}(\hat{X}, t) + \frac{ec}{E} \mathbf{P} \wedge \mathbf{B}(\hat{X}, t) - \mu_{\text{B}} \left\{ \frac{\beta c (\boldsymbol{\sigma} \wedge \mathbf{P}) \cdot \nabla \mathbf{E}}{E+mc^2} + \frac{c^2 (\boldsymbol{\sigma} \wedge \mathbf{P}) \cdot \nabla (\mathbf{P} \wedge \mathbf{B})}{E(E+mc^2)} \right\}. \quad (156)$$

(The non-commutative character of the components of  $\hat{X}$  does not cause trouble here because of the limitation to first derivatives of the fields.) Furthermore we introduce the spin operator  $\hat{s}$  (151) instead of  $\boldsymbol{\sigma}$ ; since in (155)  $\boldsymbol{\sigma}$  is only needed up to order  $e^0$  we write

$$\frac{1}{2}\hbar\boldsymbol{\sigma} = \frac{mc^2}{E} \hat{s} + \frac{c^2\mathbf{P}\mathbf{P} \cdot \hat{s}}{E(E+mc^2)}. \quad (157)$$

Substituting (156) and (157) into (155), using the Maxwell equation  $\nabla \wedge \mathbf{E} = -\partial_0 \mathbf{B}$  and introducing the abbreviations  $\boldsymbol{\beta} \equiv c\mathbf{P}/E$ ,  $\gamma \equiv (1-\boldsymbol{\beta}^2)^{-\frac{1}{2}}$  and  $\partial_0 \equiv c^{-1}\partial/\partial t$  we obtain as the equation of motion:

$$\begin{aligned}
m \frac{d\hat{v}_{\text{op}}}{dt} &\rightleftharpoons \gamma^{-2}(\mathbf{U} - \boldsymbol{\beta}\boldsymbol{\beta}) \cdot \left[ \gamma e\mathbf{E}(\hat{X}, t) + \gamma e\boldsymbol{\beta} \wedge \mathbf{B}(\hat{X}, t) \right. \\
&+ \frac{ge}{2mc} \{ (\nabla\mathbf{B}) \cdot \hat{s} + (\nabla\mathbf{E}) \cdot (\boldsymbol{\beta} \wedge \hat{s}) + \gamma^2 (\partial_0 + \boldsymbol{\beta} \cdot \nabla) \boldsymbol{\beta} \hat{s} \cdot (\mathbf{B} - \boldsymbol{\beta} \wedge \mathbf{E}) \} \\
&\left. - \frac{(g-2)e}{2mc} \gamma^2 (\partial_0 + \boldsymbol{\beta} \cdot \nabla) \{ \hat{s} \wedge (\mathbf{E} + \boldsymbol{\beta} \wedge \mathbf{B}) - \hat{s} \wedge \boldsymbol{\beta} \boldsymbol{\beta} \cdot \mathbf{E} \} \right]. \quad (158)
\end{aligned}$$

Here we have limited ourselves to the ‘upper left’ part of the matrix expression (i.e.  $\beta$  replaced by 1) which is the relevant part if expectation values for positive-energy solutions are evaluated. (Again the time and space derivations act only on the fields.)

At the right-hand side various terms which represent forces appear. (The factor  $\mathbf{U} - \boldsymbol{\beta}\boldsymbol{\beta}$  arose, because we considered the time derivative of the velocity operator. In classical theory one also encounters a similar factor in that case.) In the first place one recognizes the Lorentz force on the particle with charge  $e$ . Its velocity independent part is equal to  $e\mathbf{E}$ . The quantity  $\boldsymbol{\beta}$  is, up to order  $e^0$  and for positive-energy solutions, the Weyl transform of the velocity operator times  $c^{-1}$ , as (154) shows. Next, two terms with space derivatives of the fields  $\mathbf{E}$  and  $\mathbf{B}$  appear. The velocity independent part is the ‘Kelvin force’  $(\nabla\mathbf{B}) \cdot \hat{\mathbf{m}}$ , where  $\hat{\mathbf{m}}$  stands for the total magnetic moment  $(ge/2mc)\hat{s}$  in the Blount picture. Finally two terms with the total time derivation  $\partial_0 + \boldsymbol{\beta} \cdot \nabla$  of the fields appear. The velocity independent part is  $-\partial_0(\hat{\mathbf{m}}_a \wedge \mathbf{E})$  with  $\hat{\mathbf{m}}_a$  the anomalous magnetic moment  $\{(g-2)e/2mc\}\hat{s}$  in the Blount picture. This magnetodynamic effect is seen to contain the vector product of the electric field  $\mathbf{E}$  and the anomalous part of the magnetic moment<sup>1</sup>.

The magnetodynamic effect was discussed extensively in recent years. Some authors<sup>2</sup> found, in contrast with the result obtained, that also the normal magnetic moment (or half it) contributes to this effect. This is a consequence of the fact that their treatment was based on non-covariant position operators, such as Newton–Wigner’s or the even part of Dirac’s operator (v. problems 4 and 5)<sup>3</sup>.

The *spin* equation follows by taking the total time derivative of the spin operator (151) in the Blount picture. Using the Hamiltonian (143) we obtain for its Weyl transform

$$\begin{aligned}
\frac{d\hat{s}_{\text{op}}}{dt} &\equiv \frac{i}{\hbar} [\hat{H}_{\text{op}}, \hat{s}_{\text{op}}] + \frac{\partial\hat{s}_{\text{op}}}{\partial t} \rightleftharpoons \mu_{\text{B}} \left\{ \beta\boldsymbol{\sigma} \wedge \mathbf{B} - \frac{\beta c^2 \mathbf{P} \wedge \mathbf{B} \mathbf{P} \cdot \boldsymbol{\sigma}}{E(E+mc^2)} + \left( \frac{c\mathbf{P}}{E} \wedge \boldsymbol{\sigma} \right) \wedge \mathbf{E} \right\} \\
&+ \frac{1}{2}(g-2)\mu_{\text{B}} \left\{ \beta\boldsymbol{\sigma} \wedge \mathbf{B} + \frac{\beta \mathbf{P} \wedge \mathbf{B} \mathbf{P} \cdot \boldsymbol{\sigma}}{m(E+mc^2)} - \frac{c\mathbf{P} \boldsymbol{\sigma} \cdot \mathbf{E}}{E} + \frac{E\mathbf{P} \cdot \boldsymbol{\sigma}}{mc} - \frac{c\mathbf{P} \mathbf{P} \cdot \boldsymbol{\sigma} \mathbf{P} \cdot \mathbf{E}}{mE(E+mc^2)} \right\}, \quad (159)
\end{aligned}$$

<sup>1</sup> L. G. Suttorp and S. R. de Groot, op. cit.

<sup>2</sup> A. Conort, Compt. Rend. 266 B(1968)1184; H. Bacry, Compt. Rend. 267 B(1968)89; W. Shockley, Phys. Rev. Lett. 20(1968)343; W. Shockley and K. K. Thornber, Phys. Lett. 27 A(1968)534; J. H. Van Vleck and N. L. Huang, Phys. Lett. 28 A(1969)768.

<sup>3</sup> P. Hraskó, N. Cim. 3B(1971)213, avoids this problem by studying particles with an anomalous magnetic moment only, using the Newton–Wigner position operator.

where only terms linear in  $e$  and without derivatives of the fields have been included. Upon introduction of  $\hat{s}$  with the help of (157) the equation becomes

$$\frac{d\hat{s}_{\text{op}}}{dt} \rightleftharpoons \frac{ge}{2mc} \frac{mc^2}{E} \left\{ \beta \hat{s} \wedge \mathbf{B} + \left( \frac{c\mathbf{P}}{E} \wedge \hat{s} \right) \wedge \mathbf{E} \right\} + \frac{(g-2)e}{2mc} \left\{ \beta \frac{\mathbf{P} \cdot \hat{s}}{mE} \mathbf{P} \wedge \mathbf{B} - \frac{mc^3}{E^2} \mathbf{P} \wedge (\hat{s} \wedge \mathbf{E}) - \frac{c}{mE^2} \mathbf{P} \wedge (\mathbf{P} \wedge \mathbf{E}) \mathbf{P} \cdot \hat{s} \right\}. \quad (160)$$

Using the same abbreviations as in (158) and replacing again the matrix  $\beta$  by 1 (i.e. limiting ourselves to the part occurring in the expectation value for the positive-energy solutions) we get finally

$$\frac{d\hat{s}_{\text{op}}}{dt} \rightleftharpoons \frac{ge}{2mc} \gamma^{-1} \{ \hat{s} \wedge \mathbf{B} + (\beta \wedge \hat{s}) \wedge \mathbf{E} \} + \frac{(g-2)e}{2mc} \gamma^{-1} \{ \gamma^2 \beta \cdot \hat{s} (\mathbf{E} + \beta \wedge \mathbf{B}) - \hat{s} \beta \cdot \mathbf{E} - \gamma^2 \beta \beta \cdot \hat{s} \beta \cdot \mathbf{E} \}. \quad (161)$$

At the right-hand side various terms appear which express the torques exerted by the fields on the particle with magnetic moment. The first two terms contain the total magnetic moment  $\hat{\mathbf{m}}$ , the remaining ones the anomalous part  $\hat{\mathbf{m}}_a$  of it only. The velocity independent term is simply  $\hat{\mathbf{m}} \wedge \mathbf{B}$ .

Equations (158) and (161) are the quantum-mechanical equations of motion and of spin for a Dirac particle with both a normal and an anomalous magnetic moment moving in an external electromagnetic field. They are essentially operator equations: at the right-hand side Weyl transforms appear from which the corresponding operators might be retraced.

From the operator equations one obtains directly equations for expectation values. They contain expectation values of products of operators. In general such expectation values are not equal to the product of expectation values of the individual operators. In the *classical* limit the expectation value of a product of operators does become equal – for narrow wave packets – to the product of expectation values. Then one obtains equations for expectation values, which have precisely the same form as the corresponding equations derived in classical theory (v. (IV.162–163))<sup>1</sup>.

<sup>1</sup> Earlier discussions on the derivation of equations of classical form from quantum theory include a paper by D. M. Fradkin and R. H. Good jr. (Rev. Mod. Phys. **33**(1961) 343) on the motion of wave packets in homogeneous fields. Furthermore WKB methods have been used, for homogeneous fields, by S. I. Rubinow and J. B. Keller (Phys. Rev. **131**(1963)2789) and by K. Rafanelli and R. Schiller (Phys. Rev. **135B**(1964)279). W. G. Dixon (N. Cim. **38**(1965) 1616) employed position and spin operators without specifying the contributions due to electromagnetic potentials; he limited himself to a particle with a

## 4 The free Klein–Gordon particle

### a. The Klein–Gordon equation and its transformation properties

In this section and the following we shall derive the equation of motion for a relativistic particle without spin, i.e. a particle which is described by the Klein–Gordon equation. It will turn out that a treatment that is to a large extent analogous to the one given above may be followed. Again we shall study first the free particle before discussing the particle under the influence of an electromagnetic field.

The Klein–Gordon equation of a free particle without spin and with mass  $m$  ( $\neq 0$ ) reads in the coordinate representation

$$\left( \square - \frac{m^2 c^2}{\hbar^2} \right) \psi(\mathbf{R}, t) = 0, \quad (162)$$

with  $\square = \Delta - c^{-2} \partial^2 / \partial t^2$  the d'Alembertian and  $\psi(\mathbf{R}, t)$  the wave function. The inner product of two wave functions  $\psi_1$  and  $\psi_2$

$$\langle \psi_1 | \psi_2 \rangle \equiv \frac{i\hbar}{mc} \int \psi_1^* \overleftrightarrow{\partial}_0 \psi_2 d\mathbf{R} \equiv \frac{i\hbar}{mc^2} \int \left( \psi_1^* \frac{\partial \psi_2}{\partial t} - \frac{\partial \psi_1^*}{\partial t} \psi_2 \right) d\mathbf{R} \quad (163)$$

is defined in such a way, that it is conserved if  $\psi_1$  and  $\psi_2$  fulfil the Klein–Gordon equation. (In the following we shall consider only normalized wave functions  $\psi$ , i.e. with  $\langle \psi | \psi \rangle = 1$ .) The expectation value of an operator  $\Omega_{\text{op}}$  is defined as

$$\bar{\Omega}_{\text{op}} = \frac{i\hbar}{mc^2} \int \left( \psi^* \Omega_{\text{op}} \frac{\partial \psi}{\partial t} - \frac{\partial \psi^*}{\partial t} \Omega_{\text{op}} \psi \right) d\mathbf{R}. \quad (164)$$

The transformation properties of the wave function which leave the Klein–Gordon equation and the absolute value of the inner product (163) invariant are the following. Under *spatial translations* (6),  $\mathbf{R}' = \mathbf{R} + \boldsymbol{\varepsilon}$ ,  $t' = t$ , the wave function is invariant:

$$\psi'(\mathbf{R}', t') = \psi(\mathbf{R}, t). \quad (165)$$

normal magnetic moment in a homogeneous field. H. C. Corben (Phys. Rev. **121**(1961) 1833), M. Kolsrud (N. Cim. **39**(1965)504), E. Plahte (Suppl. N. Cim. **4**(1966)246, 291; **5**(1967)944), H. Yamasaki (Progr. Theor. Phys. **39**(1968)372) and K. Rafanelli (N. Cim. **67A**(1970)48) introduce proper time into Dirac theory without solving the difficulties of interpretation pertinent to this notion.



Under *rotations* (12),  $\mathbf{R}' = \mathbf{R} + \boldsymbol{\varepsilon} \wedge \mathbf{R}$ ,  $t' = t$ , the wave function is also invariant

$$\psi'(\mathbf{R}', t') = \psi(\mathbf{R}, t). \quad (166)$$

Under *spatial inversion* (18),  $\mathbf{R}' = -\mathbf{R}$ ,  $t' = t$ , we have once again<sup>1</sup>

$$\psi'(\mathbf{R}', t') = \psi(\mathbf{R}, t). \quad (167)$$

Under *time reversal* (22),  $\mathbf{R}' = \mathbf{R}$ ,  $t' = -t$ , the wave function undergoes an anti-linear transformation

$$\psi'(\mathbf{R}', t') = \psi^*(\mathbf{R}, t). \quad (168)$$

Finally, under *pure Lorentz transformations* (27),  $\mathbf{R}' = \mathbf{R} - \boldsymbol{\varepsilon} ct$ ,  $ct' = ct - \boldsymbol{\varepsilon} \cdot \mathbf{R}$ , we have

$$\psi'(\mathbf{R}', t') = \psi(\mathbf{R}, t). \quad (169)$$

#### b. Feshbach and Villars's formulation

The Klein-Gordon equation is a differential equation of second order in the time. It may be written in the form of a first order equation for a two-component wave function by introducing<sup>2</sup> the functions:

$$\begin{aligned} u &\equiv \frac{1}{\sqrt{2}} \left( \psi - \frac{\hbar}{imc^2} \frac{\partial \psi}{\partial t} \right), \\ v &\equiv \frac{1}{\sqrt{2}} \left( \psi + \frac{\hbar}{imc^2} \frac{\partial \psi}{\partial t} \right). \end{aligned} \quad (170)$$

With the two-component wave function

$$\Psi = \begin{pmatrix} u \\ v \end{pmatrix} \quad (171)$$

one may write the Klein-Gordon equation (162) for a free particle as

$$H_{\text{op}} \Psi = -\frac{\hbar}{i} \frac{\partial \Psi}{\partial t}, \quad (172)$$

with the Hamilton operator

$$H_{\text{op}} \equiv (\tau_3 + i\tau_2) \frac{\mathbf{P}_{\text{op}}^2}{2m} + mc^2 \tau_3, \quad (173)$$

<sup>1</sup> Phase factors are ignored, just as before, since they have no influence on the expectation values considered.

<sup>2</sup> H. Feshbach and F. Villars, Rev. Mod. Phys. 30(1958)24; cf. M. Taketani and S. Sakata, Proc. Phys. Math. Soc. Japan 22(1940)757.

where  $\tau_i$  are the Pauli matrices (52), and  $\mathbf{P}_{\text{op}}$  is the momentum operator  $(\hbar/i)\partial/\partial\mathbf{R}$ .

The inner product (163) may now be written as

$$\langle \Psi_1 | \Psi_2 \rangle \equiv \int \Psi_1^\dagger \tau_3 \Psi_2 d\mathbf{R}, \quad (174)$$

where the obelisk denotes the hermitian conjugate. This follows by insertion of the components (170) of the wave functions  $\Psi_1$  and  $\Psi_2$ . The expectation value of an operator will be defined as

$$\bar{\Omega}_{\text{op}} = \int \Psi^\dagger \tau_3 \Omega_{\text{op}} \Psi d\mathbf{R}. \quad (175)$$

This definition reduces to (164) for operators which are a multiple of the  $2 \times 2$  unit matrix. An operator has real expectation values (175) if one has

$$\Omega_{\text{op}}^\dagger = \tau_3 \Omega_{\text{op}} \tau_3. \quad (176)$$

In particular one may notice that  $H_{\text{op}}$  (173) satisfies this relation.

The transformation properties (165–169) may be expressed in terms of the new wave function  $\Psi$ . For translations (165), rotations (166) and spatial inversion (167) we get each time

$$\Psi'(\mathbf{R}', t') = \Psi(\mathbf{R}, t). \quad (177)$$

Under *translations* the expectation value of an operator changes therefore by an amount which is the expectation value of

$$\delta \Omega_{\text{op}} = \frac{i}{\hbar} \boldsymbol{\varepsilon} \cdot [\mathbf{P}_{\text{op}}, \Omega_{\text{op}}], \quad (178)$$

while under *rotations* we have

$$\delta \Omega_{\text{op}} = \frac{i}{\hbar} \boldsymbol{\varepsilon} \cdot [\mathbf{R} \wedge \mathbf{P}_{\text{op}}, \Omega_{\text{op}}]. \quad (179)$$

A vector operator is characterized by its property

$$[(\mathbf{R} \wedge \mathbf{P}_{\text{op}})^i, \Omega_{\text{op}}^j] = i\hbar \varepsilon^{ijk} \Omega_{k,\text{op}}. \quad (180)$$

Under *spatial inversion* the expectation value changes according to

$$\begin{aligned} &\int \Psi'^\dagger(\mathbf{R}', t') \tau_3 \Omega_{\text{op}} \left( \mathbf{R}', \frac{\hbar}{i} \frac{\partial}{\partial \mathbf{R}'} \right) \Psi'(\mathbf{R}', t') d\mathbf{R}' \\ &= \int \Psi^\dagger(\mathbf{R}, t) \tau_3 \Omega_{\text{op}} \left( -\mathbf{R}, -\frac{\hbar}{i} \frac{\partial}{\partial \mathbf{R}} \right) \Psi(\mathbf{R}, t) d\mathbf{R}. \end{aligned} \quad (181)$$

In particular a polar or axial vector operator satisfies the relation

$$\Omega_{\text{op}}(-\mathbf{R}, -\mathbf{P}_{\text{op}}) = \mp \Omega_{\text{op}}(\mathbf{R}, \mathbf{P}_{\text{op}}). \quad (182)$$

The transformation property of the wave function under *time reversal* follows from (168):

$$\Psi'(\mathbf{R}', t') = \Psi^*(\mathbf{R}, t), \quad (183)$$

so that the expectation value of an operator  $\Omega_{\text{op}}$  transforms according to

$$\begin{aligned} \int \Psi'^{\dagger}(\mathbf{R}', t') \tau_3 \Omega_{\text{op}} \left( \mathbf{R}', \frac{\hbar}{i} \frac{\partial}{\partial \mathbf{R}'} \right) \Psi'(\mathbf{R}', t') d\mathbf{R}' \\ = \int \Psi^{\dagger}(\mathbf{R}, t) \tilde{\Omega}_{\text{op}} \left( \mathbf{R}, -\frac{\hbar}{i} \frac{\partial}{\partial \mathbf{R}} \right) \tau_3 \Psi(\mathbf{R}, t) d\mathbf{R}, \end{aligned} \quad (184)$$

where the tilde indicates the transposed matrix.

Finally under *pure Lorentz transformations* the two-component wave function transforms as

$$\Psi'(\mathbf{R}', t') = \left\{ 1 - \frac{1}{2}(\tau_3 + i\tau_2) \frac{\boldsymbol{\varepsilon} \cdot \mathbf{P}_{\text{op}}}{mc} \right\} \Psi(\mathbf{R}, t), \quad (185)$$

as follows from (169) with (170) and (171). The change of the expectation value of an operator  $\Omega_{\text{op}}$  under pure Lorentz transformations may be found now by proceeding along similar lines as followed in (29–33). One finds that the change of the expectation value is given by the expectation value of the operator

$$\delta \Omega_{\text{op}} = \frac{i}{\hbar} \boldsymbol{\varepsilon} \cdot [N_{\text{op}} - ct \mathbf{P}_{\text{op}}, \Omega_{\text{op}}], \quad (186)$$

where the operator  $N_{\text{op}}$  stands for

$$N_{\text{op}} \equiv \frac{1}{2} c^{-1} \{ \mathbf{R}, H_{\text{op}} \}. \quad (187)$$

The curly brackets indicate an anticommutator and  $H_{\text{op}}$  is given by (173).

#### c. Covariance requirements on the position operator

The position operator  $\mathbf{X}_{\text{op}}$  for the Klein–Gordon particle will be obtained by imposing a number of conditions. We require in the first place that it be a polar vector operator with the usual property under translations:

$$[\mathbf{P}_{\text{op}}, \mathbf{X}_{\text{op}}] = \frac{\hbar}{i} \mathbf{U}, \quad (188)$$

$$[(\mathbf{R} \wedge \mathbf{P}_{\text{op}})^i, X_{\text{op}}^j] = i \hbar \varepsilon^{ijk} X_{k, \text{op}}, \quad (189)$$

$$\mathbf{X}_{\text{op}}(-\mathbf{R}, -\mathbf{P}_{\text{op}}) = -\mathbf{X}_{\text{op}}(\mathbf{R}, \mathbf{P}_{\text{op}}), \quad (190)$$

where (178), (180) and (182) have been used. As to its time reversal property we require that the expectation value of the position operator be invariant, i.e., according to (184),

$$\mathbf{X}_{\text{op}}(\mathbf{R}, -\mathbf{P}_{\text{op}}) = \tau_3 \tilde{\mathbf{X}}_{\text{op}}(\mathbf{R}, \mathbf{P}_{\text{op}}) \tau_3. \quad (191)$$

For the pure Lorentz transformation character we postulate in view of (44) (which is valid for any spin) and (186)

$$[N_{\text{op}}^i, X_{\text{op}}^j] = \frac{1}{2} c^{-1} \{ X_{\text{op}}^i, [H_{\text{op}}, X_{\text{op}}^j] \}, \quad (192)$$

where we applied the translation property (188).

#### d. Transformation to even form of the Hamilton operator; the position operator

The Feshbach–Villars Hamiltonian (173) contains the odd matrix  $\tau_2$ . As a consequence the wave equation (172) consists of two coupled differential equations. They may be uncoupled by performing a transformation<sup>1</sup> which is the analogue of the Pryce–Foldy–Wouthuysen transformation for the Dirac particle. If one transforms the wave function according to

$$\hat{\Psi} = U_{\text{op}} \Psi, \quad (193)$$

the operators  $\Omega_{\text{op}}$  should transform in such a way that the expectation values are invariant, i.e. as a consequence of (175),

$$\int \hat{\Psi}_1^{\dagger} \tau_3 \hat{\Omega}_{\text{op}} \hat{\Psi}_2 d\mathbf{R} = \int \Psi_1^{\dagger} \tau_3 \Omega_{\text{op}} \Psi_2 d\mathbf{R}, \quad (194)$$

so that, with (193), we have

$$\hat{\Omega}_{\text{op}} = \tau_3 (U_{\text{op}}^{\dagger})^{-1} \tau_3 \Omega_{\text{op}} U_{\text{op}}^{-1}. \quad (195)$$

In particular choosing  $\Omega_{\text{op}}$  as the unit operator and requiring that  $\hat{\Omega}_{\text{op}}$  be the unit operator as well (so that the inner product (174) is invariant) one has

$$1 = \tau_3 (U_{\text{op}}^{\dagger})^{-1} \tau_3 U_{\text{op}}^{-1}, \quad (196)$$

or equivalently

$$U_{\text{op}} = \tau_3 (U_{\text{op}}^{\dagger})^{-1} \tau_3, \quad (197)$$

<sup>1</sup> H. Feshbach and F. Villars, op. cit.

so that (195) may be written as

$$\hat{Q}_{\text{op}} = U_{\text{op}} \Omega_{\text{op}} U_{\text{op}}^{-1}. \quad (198)$$

The Hamiltonian, which governs the time behaviour of  $\hat{\Psi}$ , follows from (172) and (193):

$$\hat{H}_{\text{op}} = U_{\text{op}} H_{\text{op}} U_{\text{op}}^{-1} - \frac{\hbar}{i} \frac{\partial U_{\text{op}}}{\partial t} U_{\text{op}}^{-1}. \quad (199)$$

(One should note that this transformation of the Hamiltonian is of course not of the type (198); only if  $U_{\text{op}}$  is independent of the time – as it will turn out to be in the present field-free case – this expression reduces to its first term.)

The Hamiltonian  $H_{\text{op}}$  (173) may be diagonalized with the help of an operator  $U_{\text{op}}$  which is such that its inverse  $U_{\text{op}}^{-1}$  contains in its columns the eigenvectors of  $H_{\text{op}}$ . Then one finds that a possible choice for  $U_{\text{op}}$  is:

$$U_{\text{op}} = \frac{1}{2}(1 + \tau_1) \left( \frac{E_{\text{op}}}{mc^2} \right)^{\frac{1}{2}} + \frac{1}{2}(1 - \tau_1) \left( \frac{mc^2}{E_{\text{op}}} \right)^{\frac{1}{2}}, \quad (200)$$

where the energy operator is

$$E_{\text{op}} \equiv (\mathbf{P}_{\text{op}}^2 c^2 + m^2 c^4)^{\frac{1}{2}}. \quad (201)$$

The form (200) satisfies (197). Indeed the transformed Hamiltonian (199), that follows from (173) by applying the time-independent transformation operator (200), is now

$$\hat{H}_{\text{op}} = \tau_3 E_{\text{op}} \quad (202)$$

and has thus diagonal form. Hence the positive- and negative-energy solutions in this new picture (indicated by circumflexes) are no longer mixed. For that reason only that part of the operators for physical quantities that is even in the new picture comes into play if one considers its expectation value for positive- (or negative-) energy solutions.

The even part of the position operator, which will be denoted as  $\hat{X}_{\text{op}}$  in the new picture, follows from the requirements (188–192). From the requirements (188) and (189) alone – translation and rotation covariance – one has the general form

$$\hat{X}_{\text{op}} = \mathbf{R} + f_1(E_{\text{op}}) \mathbf{P}_{\text{op}} + f_2(E_{\text{op}}) \tau_3 \mathbf{P}_{\text{op}}, \quad (203)$$

with arbitrary functions  $f_1$  and  $f_2$ . The requirement (190) about spatial inversion does not restrict (203) any further. The requirement of time reversal (191) makes both  $f_1$  and  $f_2$  vanish. Thus the even part of the position opera-

tor in the new picture is found to be

$$\hat{X}_{\text{op}} = \mathbf{R}. \quad (204)$$

One should still check whether this result satisfies the Lorentz covariance condition (192) (with circumflexes). To that end we write first the transformed coordinate

$$\hat{\mathbf{R}}_{\text{op}} \equiv U_{\text{op}} \mathbf{R} U_{\text{op}}^{-1} = \mathbf{R} + \xi_{\text{op}}, \quad (205)$$

with the latter quantity given by

$$\xi_{\text{op}} = -\frac{\hbar}{i} U_{\text{op}} \frac{\partial U_{\text{op}}^{-1}}{\partial \mathbf{P}_{\text{op}}} = \frac{\hbar}{i} \frac{\partial U_{\text{op}}}{\partial \mathbf{P}_{\text{op}}} U_{\text{op}}^{-1} \quad (206)$$

or explicitly, with (200) inserted,

$$\xi_{\text{op}} = \frac{\hbar c^2 \mathbf{P}_{\text{op}}}{2iE_{\text{op}}} \tau_1. \quad (207)$$

Then the operator  $\hat{N}_{\text{op}}$  (187) becomes with (202), (205) and (207):

$$\hat{N}_{\text{op}} = \frac{1}{2} c^{-1} \tau_3 \{ \mathbf{R}, E_{\text{op}} \}. \quad (208)$$

Substituting this expression, (202) and (204) into (192) with circumflexes, one finds an identity, so that indeed the Lorentz covariance condition is satisfied.

We note that the position operator (204) reads in the original, Feshbach-Villars picture

$$\mathbf{X}_{\text{op}} = \mathbf{R} - \frac{\hbar c^2 \mathbf{P}_{\text{op}}}{2iE_{\text{op}}} \tau_1. \quad (209)$$

A few remarks may be made about the position operator obtained. In the first place we note that its components commute (in contrast with the components of the position operator for the Dirac particle). Furthermore the orbital angular momentum  $\mathbf{R} \wedge \mathbf{P}_{\text{op}}$ , which according to (179) is the generator of rotations, may be written as the vector product  $\mathbf{X}_{\text{op}} \wedge \mathbf{P}_{\text{op}}$  of the position operator  $\mathbf{X}_{\text{op}}$  and the momentum operator  $\mathbf{P}_{\text{op}}$ , as follows from (209).

The position operator found here is the same as the operator obtained by Newton and Wigner<sup>1</sup>, as may be checked by translating it into the momentum representation, which they employ.

<sup>1</sup> T. D. Newton and E. P. Wigner, *op. cit.*

## 5 The Klein–Gordon particle in a field

### a. Invariance properties

The wave function for the Klein–Gordon particle with charge  $e$  in an external electromagnetic field, described by the four-potential  $A^\mu = (\varphi, \mathbf{A})$  satisfies the equation

$$\left\{ \left( \partial_\mu - \frac{ie}{\hbar c} A_\mu \right) \left( \partial^\mu - \frac{ie}{\hbar c} A^\mu \right) - \frac{m^2 c^2}{\hbar^2} \right\} \psi(\mathbf{R}, t) = 0. \quad (210)$$

The transformation properties (165–169) of the wave function remain valid in this case if one transforms the four-potential in the right way, i.e. as a four-vector under Lorentz transformation and as  $(\varphi'(\mathbf{R}', t'), \mathbf{A}'(\mathbf{R}', t')) = (\varphi(\mathbf{R}, t), -\mathbf{A}(\mathbf{R}, t))$  both under spatial inversion and time reversal.

The Klein–Gordon equation (210) for a particle in an external field may be transformed by employing an artifice, similar to that for the free particle. In fact if one defines

$$\begin{aligned} u &= \frac{1}{\sqrt{2}} \left\{ \psi - \frac{\hbar}{imc^2} \left( \frac{\partial}{\partial t} + \frac{ie}{\hbar} \varphi \right) \psi \right\}, \\ v &= \frac{1}{\sqrt{2}} \left\{ \psi + \frac{\hbar}{imc^2} \left( \frac{\partial}{\partial t} + \frac{ie}{\hbar} \varphi \right) \psi \right\} \end{aligned} \quad (211)$$

and uses (171), one obtains for (210) an equation of the form (172), but with the Hamiltonian<sup>1</sup>

$$H_{\text{op}} = (\tau_3 + i\tau_2) \frac{\pi_{\text{op}}^2}{2m} + mc^2 \tau_3 + e\varphi, \quad (212)$$

where we introduced the abbreviation

$$\pi_{\text{op}} \equiv \mathbf{P}_{\text{op}} - \frac{e}{c} \mathbf{A}. \quad (213)$$

Let us study the invariance properties of expectation values for operators that depend not only on the coordinate and momentum operators but also on the potentials.

Under *translations* (6) one finds that the expectation value of an operator changes by an amount which is the expectation value of the operator

$$\delta\Omega_{\text{op}} = \frac{i}{\hbar} \boldsymbol{\varepsilon} \cdot [\mathbf{P}_{\text{op}}, \Omega_{\text{op}}] + \Omega_{\text{op}}(\mathbf{R}, \mathbf{P}_{\text{op}}, \mathbf{A} - \boldsymbol{\varepsilon} \cdot \nabla \mathbf{A}, \varphi - \boldsymbol{\varepsilon} \cdot \nabla \varphi) - \Omega_{\text{op}}(\mathbf{R}, \mathbf{P}_{\text{op}}, \mathbf{A}, \varphi), \quad (214)$$

<sup>1</sup> H. Feshbach and F. Villars, op. cit.

as follows from (96) and (177). If one limits oneself to terms with the potentials but without their derivatives this expression reduces to

$$\delta\Omega_{\text{op}} = \frac{i}{\hbar} \boldsymbol{\varepsilon} \cdot [\mathbf{P}_{\text{op}}, \Omega_{\text{op}}]. \quad (215)$$

Under *rotations* (12), the change of expectation values is governed by the operator

$$\begin{aligned} \delta\Omega_{\text{op}} &= \frac{i}{\hbar} \boldsymbol{\varepsilon} \cdot [\mathbf{R} \wedge \mathbf{P}_{\text{op}}, \Omega_{\text{op}}] + \Omega_{\text{op}}(\mathbf{R}, \mathbf{P}_{\text{op}}, \mathbf{A} + \boldsymbol{\varepsilon} \wedge \mathbf{A} - (\boldsymbol{\varepsilon} \wedge \mathbf{R}) \cdot \nabla \mathbf{A}, \\ &\quad \varphi - (\boldsymbol{\varepsilon} \wedge \mathbf{R}) \cdot \nabla \varphi) - \Omega_{\text{op}}(\mathbf{R}, \mathbf{P}_{\text{op}}, \mathbf{A}, \varphi), \end{aligned} \quad (216)$$

as follows from (99) and (177). Up to potentials only it becomes

$$\delta\Omega_{\text{op}} = \frac{i}{\hbar} \boldsymbol{\varepsilon} \cdot [\mathbf{R} \wedge \mathbf{P}_{\text{op}}, \Omega_{\text{op}}] + (\boldsymbol{\varepsilon} \wedge \mathbf{A}) \cdot \frac{\partial \Omega_{\text{op}}}{\partial \mathbf{A}}. \quad (217)$$

If the operator  $\Omega_{\text{op}}$  is a vector operator, it satisfies the relation

$$[(\mathbf{R} \wedge \mathbf{P}_{\text{op}})^i, \Omega_{\text{op}}^j] - i\hbar \varepsilon^{imn} A_m \frac{\partial \Omega_{\text{op}}^j}{\partial A^n} = i\hbar \varepsilon^{ijk} \Omega_{k,\text{op}}. \quad (218)$$

A particular case of (217) arises if the operator  $\Omega_{\text{op}}$  is independent of  $\varphi$  and depends on  $\mathbf{A}$  only in the combination  $\pi_{\text{op}}$  (213). Then (217) reads

$$\delta\Omega_{\text{op}} = \frac{i}{\hbar} \boldsymbol{\varepsilon} \cdot [\mathbf{R} \wedge \pi_{\text{op}}, \Omega_{\text{op}}]. \quad (219)$$

Under *spatial inversion* (18) the expectation value in the new frame is the expectation value of

$$\Omega_{\text{op}}(-\mathbf{R}, -\mathbf{P}_{\text{op}}, -\mathbf{A}, \varphi), \quad (220)$$

as follows from (105) and (177). In particular a polar or an axial vector operator is characterized by

$$\Omega_{\text{op}}(-\mathbf{R}, -\mathbf{P}_{\text{op}}, -\mathbf{A}, \varphi) = \mp \Omega_{\text{op}}(\mathbf{R}, \mathbf{P}_{\text{op}}, \mathbf{A}, \varphi). \quad (221)$$

Under *time reversal* (22) the expectation value in the new frame is the expectation value of

$$\tau_3 \tilde{\Omega}_{\text{op}}(\mathbf{R}, -\mathbf{P}_{\text{op}}, -\mathbf{A}, \varphi) \tau_3, \quad (222)$$

where we have used (108) and (183).

Under *pure Lorentz transformations* (27) the two-component wave function transforms in a way that is slightly different from the transformation

(185) for the free particle case, namely

$$\Psi'(\mathbf{R}', t') = \left\{ 1 - \frac{1}{2}(\tau_3 + i\tau_2) \frac{\boldsymbol{\varepsilon} \cdot \boldsymbol{\pi}_{\text{op}}}{mc} \right\} \Psi(\mathbf{R}, t), \quad (223)$$

as follows from (169) and the definitions (211) (note that the latter contain the scalar potential which transforms also, and thus yield a term with the vector potential). For the expectation value of an operator in the new frame one finds, by a reasoning which is analogous to that of (29–33), an expression which differs from that in the old frame by a quantity which is the expectation value of the operator

$$\delta\Omega_{\text{op}} = \frac{i}{\hbar} \boldsymbol{\varepsilon} \cdot [N_{\text{op}} - ct\mathbf{P}_{\text{op}}, \Omega_{\text{op}}] + \Omega_{\text{op}} \left( \mathbf{R}, \mathbf{P}_{\text{op}}, A - \boldsymbol{\varepsilon}\varphi + ct\boldsymbol{\varepsilon} \cdot \nabla A + c^{-1} \boldsymbol{\varepsilon} \cdot \mathbf{R} \frac{\partial A}{\partial t}, \right. \\ \left. \varphi - \boldsymbol{\varepsilon} \cdot \mathbf{A} + ct\boldsymbol{\varepsilon} \cdot \nabla\varphi + c^{-1} \boldsymbol{\varepsilon} \cdot \mathbf{R} \frac{\partial\varphi}{\partial t} \right) - \Omega_{\text{op}}(\mathbf{R}, \mathbf{P}_{\text{op}}, A, \varphi), \quad (224)$$

where (109) has been used. Here  $N_{\text{op}}$  is given by (187), but with the Hamiltonian (212). Up to terms with the potentials this expression reduces to

$$\delta\Omega_{\text{op}} = \frac{i}{\hbar} \boldsymbol{\varepsilon} \cdot [N_{\text{op}} - ct\mathbf{P}_{\text{op}}, \Omega_{\text{op}}] - \boldsymbol{\varepsilon} \cdot \frac{\partial\Omega_{\text{op}}}{\partial A} \varphi - \frac{\partial\Omega_{\text{op}}}{\partial\varphi} \boldsymbol{\varepsilon} \cdot \mathbf{A}. \quad (225)$$

If  $\Omega_{\text{op}}$  depends only on  $\mathbf{R}$  and  $\boldsymbol{\pi}_{\text{op}}$ , this expression becomes

$$\delta\Omega_{\text{op}} = \frac{i}{\hbar} \boldsymbol{\varepsilon} \cdot [N_{\text{op}}^{(\varphi)} - ct\mathbf{P}_{\text{op}}, \Omega_{\text{op}}] \quad (226)$$

with the definition

$$N_{\text{op}}^{(\varphi)} \equiv \frac{1}{2} c^{-1} \{ \mathbf{R}, H_{\text{op}} - e\varphi \}, \quad (227)$$

where we used (187).

### b. Covariance requirements on the position operator

Just as in the field-free case (section 4c) we shall list the covariance requirements for the position operator, in which we now include terms with the potentials.

The *translation* property remains of the form (188), while the *rotation* and *spatial inversion* properties follow by stipulating that the position operator be a polar vector:

$$[(\mathbf{R} \wedge \mathbf{P}_{\text{op}})^i, X_{\text{op}}^j] - i\hbar \varepsilon^{imn} A_m \frac{\partial X_{\text{op}}^j}{\partial A_n} = i\hbar \varepsilon^{ijk} X_{k,\text{op}}, \quad (228)$$

$$X_{\text{op}}(-\mathbf{R}, -\mathbf{P}_{\text{op}}, -A, \varphi) = -X_{\text{op}}(\mathbf{R}, \mathbf{P}_{\text{op}}, A, \varphi) \quad (229)$$

(cf. (218) and (221)). *Time reversal* invariance of the position operator implies (cf. (222))

$$X_{\text{op}}(\mathbf{R}, -\mathbf{P}_{\text{op}}, -A, \varphi) = \tau_3 \tilde{X}_{\text{op}}(\mathbf{R}, \mathbf{P}_{\text{op}}, A, \varphi) \tau_3. \quad (230)$$

As to the *Lorentz covariance* we require the relation

$$[N_{\text{op}}^i, X_{\text{op}}^j] - \frac{\hbar}{i} \left( \frac{\partial X_{\text{op}}^j}{\partial A_i} \varphi + \frac{\partial X_{\text{op}}^j}{\partial\varphi} A^i \right) = \frac{1}{2} c^{-1} \{ X_{\text{op}}^i, [H_{\text{op}}, X_{\text{op}}^j] \}, \quad (231)$$

which follows from (44) and (225).

### c. The transformed Hamilton operator

The Hamilton operator (212) which contains the odd matrix  $\tau_2$  may be brought into even form by means of two successive transformations. In the first place we employ a transformation operator  $U_{1,\text{op}}$  of which the Weyl transform is analogous to the Weyl transform of (200):

$$U_{1,\text{op}} \rightleftharpoons \frac{1}{2}(1 + \tau_1) \left( \frac{E_\pi}{mc^2} \right)^{\frac{1}{2}} + \frac{1}{2}(1 - \tau_1) \left( \frac{mc^2}{E_\pi} \right)^{\frac{1}{2}} \equiv U_1. \quad (232)$$

Here we used the abbreviation  $E_\pi$  (134) with  $\pi = \mathbf{p} - (e/c)\mathbf{A}$  the Weyl transform of  $\boldsymbol{\pi}_{\text{op}}$  (213). Then, since the Weyl transform of  $H_{\text{op}}$  (212) is

$$H_{\text{op}} \rightleftharpoons (\tau_3 + i\tau_2) \frac{\pi^2}{2m} + mc^2 \tau_3 + e\varphi \equiv H, \quad (233)$$

one finds up to terms with the derivatives of the potentials

$$U_{1,\text{op}} H_{\text{op}} \tau_3 U_{1,\text{op}}^\dagger \tau_3 \rightleftharpoons U_1 H \tau_3 U_1^\dagger \tau_3 \\ + \frac{ie\hbar}{2c} \varepsilon_{ijk} \frac{\partial U}{\partial P_i} \frac{\partial H}{\partial P_j} \tau_3 U^\dagger \tau_3 B^k + \frac{ie\hbar}{2c} \varepsilon_{ijk} U \frac{\partial H}{\partial P_i} \tau_3 \frac{\partial U^\dagger}{\partial P_j} \tau_3 B^k \\ + \frac{ie\hbar}{2c} \varepsilon_{ijk} \frac{\partial U}{\partial P_i} H \tau_3 \frac{\partial U^\dagger}{\partial P_j} \tau_3 B^k \\ - \frac{ie\hbar}{2} \frac{\partial U}{\partial P_i} \frac{\partial\varphi}{\partial R^i} \tau_3 U^\dagger \tau_3 + \frac{ie\hbar}{2} U \frac{\partial\varphi}{\partial R_i} \tau_3 \frac{\partial U^\dagger}{\partial P^i} \tau_3 \quad (234)$$

with  $U$  the Weyl transform of (200). Apart from the matrices  $\tau_3$  this expression is formally identical with (135). The operator  $U_{1,\text{op}}$  fulfils the relation (196) since, up to terms with the derivatives of the potentials:

$$U_{1,\text{op}} \tau_3 U_{1,\text{op}}^\dagger \tau_3 \rightleftharpoons U_1 \tau_3 U_1^\dagger \tau_3 + \frac{ie\hbar}{2c} \varepsilon_{ijk} \frac{\partial U}{\partial P_i} \tau_3 \frac{\partial U^\dagger}{\partial P_j} \tau_3 B^k = 1, \quad (235)$$

where we used the explicit expression (232) to show that the first term in the middle member is equal to 1, while the vanishing of the last term in the middle member follows from (206) with (207). This result shows that  $\tau_3 U_{1,op}^\dagger \tau_3$  is equal to  $U_{1,op}^{-1}$ . Substituting (232), (233), (202), (206) and (207) into the right-hand side of (234) we get

$$U_{1,op} H_{op} U_{1,op}^{-1} \rightleftharpoons \tau_3 E_\pi + e\varphi + e \frac{\partial \varphi}{\partial \mathbf{R}} \cdot \boldsymbol{\xi}. \quad (236)$$

Since the time derivative of the transformed wave function is determined by (199), we also need  $\partial U_{1,op}/\partial t$  of which the Weyl transform is  $-(e/c)(\partial U/\partial \mathbf{p}) \cdot (\partial A/\partial t)$  (up to terms linear in  $e$  and without second derivatives of the potentials), as follows from (232). Therefore we find

$$U_{1,op} H U_{1,op}^{-1} - \frac{\hbar}{i} \frac{\partial U_{1,op}}{\partial t} U_{1,op}^{-1} \rightleftharpoons \tau_3 E_\pi + e\varphi - e \mathbf{E} \cdot \boldsymbol{\xi}. \quad (237)$$

A second transformation with the operator

$$U_{2,op} \rightleftharpoons 1 - \frac{e}{2E} \tau_3 \mathbf{E} \cdot \boldsymbol{\xi}, \quad (238)$$

which fulfils (196) (up to terms linear in  $e$ ), brings the Hamiltonian to the even form

$$\begin{aligned} \hat{H}_{op} &\equiv U_{2,op} U_{1,op} H_{op} U_{1,op}^{-1} U_{2,op}^{-1} - \frac{\hbar}{i} \frac{\partial (U_{2,op} U_{1,op})}{\partial t} U_{1,op}^{-1} U_{2,op}^{-1} \\ &\rightleftharpoons \tau_3 E_\pi + e\varphi, \end{aligned} \quad (239)$$

up to terms linear in  $e$  and without second derivatives of the potentials. This result shows that the transformed Hamiltonian contains only terms with the potentials and not with the fields (although in the derivation terms with the derivatives of the potentials have been taken into account). This situation is different from that of the Dirac particle, as (143) shows.

#### d. The position operator and the equation of motion

From the translation, rotation, spatial inversion, time reversal and Lorentz covariance properties (188) and (228–231), it follows that the part of the position operator that is even in the new picture is, up to terms with the potentials,

$$\hat{X}_{op} \rightleftharpoons \mathbf{R}. \quad (240)$$

or, if one transforms back to the original picture,

$$\mathbf{X}_{op} \rightleftharpoons \mathbf{R} - \frac{\hbar c^2 \boldsymbol{\pi}}{2iE_\pi^2} \tau_1 \quad (241)$$

(cf. (209) for the field-free case).

The time derivative of the expectation value of the position operator (240) is the expectation value of the velocity operator

$$\hat{\mathbf{v}}_{op} \equiv \frac{d\hat{X}_{op}}{dt} \equiv \frac{i}{\hbar} [\hat{H}_{op}, \hat{X}_{op}]. \quad (242)$$

This may be seen by writing for an arbitrary operator  $\hat{\Omega}_{op}$

$$\frac{\partial}{\partial t} \int \hat{\Psi}^\dagger \tau_3 \hat{\Omega}_{op} \hat{\Psi} d\mathbf{R} = \int \hat{\Psi}^\dagger \tau_3 \left\{ \frac{i}{\hbar} [\hat{H}_{op}, \hat{\Omega}_{op}] + \frac{\partial \hat{\Omega}_{op}}{\partial t} \right\} \hat{\Psi} d\mathbf{R}, \quad (243)$$

as follows from (172) with circumflexes and the fact that the Hamiltonian (239) commutes with  $\tau_3$ . From (239) and (240) one finds for (242):

$$\hat{\mathbf{v}}_{op} \rightleftharpoons \tau_3 \frac{c^2 \boldsymbol{\pi}}{E_\pi}. \quad (244)$$

For the second time derivative of  $\hat{X}_{op}$  one finds with (239):

$$\frac{d^2 \hat{X}_{op}}{dt^2} \equiv \frac{d\hat{\mathbf{v}}_{op}}{dt} \equiv \frac{i}{\hbar} [\hat{H}_{op}, \hat{\mathbf{v}}_{op}] + \frac{\partial \hat{\mathbf{v}}_{op}}{\partial t} \rightleftharpoons \frac{c^2}{E} \left( \mathbf{U} - \frac{c^2 \mathbf{P} \mathbf{P}}{E^2} \right) \cdot \left( \tau_3 e \mathbf{E} + e \frac{c \mathbf{P}}{E} \wedge \mathbf{B} \right). \quad (245)$$

If only the positive energy solutions are considered, one may replace  $\tau_3$  by 1. Then (245) becomes

$$m \frac{d\hat{\mathbf{v}}_{op}}{dt} \rightleftharpoons \gamma^{-1} (\mathbf{U} - \boldsymbol{\beta} \boldsymbol{\beta}) \cdot (e \mathbf{E} + e \boldsymbol{\beta} \wedge \mathbf{B}), \quad (246)$$

where we introduced the abbreviations  $\boldsymbol{\beta} \equiv c\mathbf{P}/E$  and  $\gamma \equiv (1 - \boldsymbol{\beta}^2)^{-\frac{1}{2}}$ . Up to order  $e^0$  and for positive energy solutions  $\boldsymbol{\beta}$  is the Weyl transform of  $c^{-1}$  times the velocity operator.

The right-hand side of (246) contains the Lorentz force, but no terms with derivatives of the fields, although such terms with first derivatives have been taken into account in the derivation. (For the Dirac particle they did occur, as (158) shows.) The factor  $\mathbf{U} - \boldsymbol{\beta} \boldsymbol{\beta}$  is a consequence of the fact that we studied the time derivative of the velocity operator: in classical theory one encounters a factor of the same type.

The same general remarks on the connexion with classical theory as made at the end of section 3 for the Dirac particle apply also here.

## APPENDIX

## On covariance properties of physical quantities for the Dirac and Klein-Gordon particles

### a. The Dirac equation in covariant notation

The Dirac equation (1) with (2) for a free particle may be written in covariant form, by introducing the matrices  $\gamma^0 = -i\beta$  and  $\gamma = -i\beta\alpha$ , which fulfil the anticommutation relations

$$\{\gamma^\mu, \gamma^\nu\} = 2g^{\mu\nu}, \quad (\text{A1})$$

where the metric tensor  $g^{\mu\nu}$  has components  $g^{00} = -1$ ,  $g^{ii} = 1$  ( $i = 1, 2, 3$ ) and the others zero. Since  $\alpha$  and  $\beta$  are hermitian,  $\gamma^0$  is anti-hermitian and  $\gamma$  hermitian. By multiplication of the Dirac equation (1) with (2) by  $\beta/\hbar c$  one obtains the form

$$\left( \gamma^\mu \partial_\mu + \frac{mc}{\hbar} \right) \psi = 0, \quad (\text{A2})$$

with  $\partial_\mu = \partial/\partial R^\mu$ . The covariance properties of this equation follow by considering an infinitesimal Poincaré transformation

$$R'^\mu = (\delta_\nu^\mu + \varepsilon_\nu^\mu) R^\nu + \eta^\mu \quad (\text{A3})$$

with  $\eta^\mu$  an infinitesimal four-vector and  $\varepsilon^{\mu\nu}$  an infinitesimal antisymmetric four-tensor. The Dirac equation (A2) is covariant with respect to the Poincaré group if one transforms the wave function as

$$\psi'(\mathbf{R}', t') = (1 + \frac{1}{4} i \varepsilon^{\mu\nu} \sigma_{\mu\nu}) \psi(\mathbf{R}, t) \quad (\text{A4})$$

with  $\sigma^{\mu\nu} \equiv -\frac{1}{2} i [\gamma^\mu, \gamma^\nu]$ . Indeed the covariance of the Dirac equation follows, if one substitutes this expression and the transformed four-derivative (which follows from (A3)) into the equation (A2) written with primes and if use is made of the commutation rule

$$[\gamma^\mu, \frac{1}{4} i \varepsilon^{\lambda\rho} \sigma_{\lambda\rho}] = \varepsilon^{\mu\lambda} \gamma_\lambda. \quad (\text{A5})$$

In particular if  $\varepsilon^{ij} = -\varepsilon^{jk} \varepsilon_k$  (with  $\varepsilon^{ijk}$  the antisymmetric unit tensor and  $\varepsilon$  an infinitesimal three-vector),  $\varepsilon^{i0} = 0$  and  $\eta^\mu = 0$  one finds for (A3) the expression (12) and for (A4) the expression (13). The latter fact follows because  $\varepsilon^{ij} \sigma_{ij} = -\varepsilon^{ijk} \varepsilon_k \sigma_{ij} = -2\boldsymbol{\varepsilon} \cdot \boldsymbol{\sigma}$  with  $\boldsymbol{\sigma} = -\frac{1}{2} i \boldsymbol{\gamma} \wedge \boldsymbol{\gamma} = -\frac{1}{2} i \boldsymbol{\alpha} \wedge \boldsymbol{\alpha}$ .

In the special case  $\varepsilon_{,0}^i = \varepsilon_{,i}^0 = -\varepsilon^i$  (with an infinitesimal three-vector  $\boldsymbol{\varepsilon}$ ),  $\varepsilon^{ij} = 0$  and  $\eta^\mu = 0$  one recovers (27) from (A3), and (28) from (A4).

One may also prove the invariance of the Dirac equation under spatial inversion

$$t' = t, \quad \mathbf{R}' = -\mathbf{R}. \quad (\text{A6})$$

Indeed with the transformation of the wave function

$$\psi'(\mathbf{R}', t') = i\gamma^0 \psi(\mathbf{R}, t) \quad (\text{A7})$$

(instead of  $i\gamma^0 = \beta$  one might as well use  $\gamma^0$  times a different phase factor) one finds that the Dirac equation is valid with primes throughout.

Finally the Dirac equation is invariant under time reversal

$$t' = -t, \quad \mathbf{R}' = \mathbf{R}. \quad (\text{A8})$$

With the anti-linear transformation

$$\psi'(\mathbf{R}', t') = T\psi^*(\mathbf{R}, t) \quad (\text{A9})$$

(the asterisk indicates the complex conjugate), where  $T$  is a matrix such that

$$T^{-1} \gamma^0 T = -\gamma^{0*}, \quad T^{-1} \gamma^i T = \gamma^{i*}, \quad (\text{A10})$$

one finds that the Dirac equation is valid for primed quantities. (In the Pauli representation one has  $\gamma^0 = -i\rho_3$  and  $\gamma = \rho_2 \boldsymbol{\sigma}$ , so that  $\boldsymbol{\alpha} = \rho_1 \boldsymbol{\sigma}$  and  $\beta = \rho_3$ ; one finds from (A10) that a possible choice for  $T$  is  $\sigma_2$ .)

The Dirac equation for a particle with an anomalous magnetic moment (1) with (93) becomes in covariant notation

$$\left\{ \gamma^\mu \left( \partial_\mu - \frac{ie}{\hbar c} A_\mu \right) + \frac{mc}{\hbar} - \frac{(g-2)e}{8mc^2} \sigma^{\mu\nu} F_{\mu\nu} \right\} \psi = 0. \quad (\text{A11})$$

The covariance of this equation follows by using the same arguments as above.

### b. Local covariance and Klein's theorem

From the transformation character of the four-component wave function  $\psi$  under pure Lorentz transformations we shall prove the following lemma:

Let  $\Omega_{\text{op}}^{v_1 \dots v_n}$  (with  $v_1, \dots, v_n$  assuming the values 0, 1, 2, 3) be a set of operators depending on Dirac matrices and the momentum operator  $\mathbf{P}_{\text{op}} = (\hbar/i)\partial/\partial\mathbf{R}$ . Then the quantity

$$\bar{\psi}(\mathbf{R}) \gamma^\mu \Omega_{\text{op}}^{v_1 \dots v_n}(\mathbf{P}_{\text{op}}) \psi(\mathbf{R}) \quad (\text{A12})$$

(with  $\bar{\psi} \equiv \psi^\dagger \gamma^0$ ) is – for all solutions  $\psi$  of the Dirac equation for a free particle – a local tensor density under pure Lorentz transformations if and only if the operator relation:

$$[N_{\text{op}}^i, \Omega_{\text{op}}^{v_1 \dots v_n}] = c^{-1} R^i [H_{\text{op}}, \Omega_{\text{op}}^{v_1 \dots v_n}] + i\hbar \sum_{j=1}^n (g^{iv_j} \Omega_{\text{op}}^{v_1 \dots v_{j-1} 0 v_{j+1} \dots v_n} - g^{0v_j} \Omega_{\text{op}}^{v_1 \dots v_{j-1} iv_{j+1} \dots v_n}), \quad (\text{A13})$$

(with  $N_{\text{op}}$  given in (34) as  $\frac{1}{2}c^{-1}\{\mathbf{R}, H_{\text{op}}\}$ ) holds true.

*Proof:* Under the pure Lorentz transformation (27) the quantity (A12) is, according to (28), transformed to

$$\begin{aligned} & \bar{\psi}'(R') \gamma^\mu \Omega_{\text{op}}^{v_1 \dots v_n}(\mathbf{P}'_{\text{op}}) \psi'(R') \\ &= \bar{\psi}(R) (1 + \frac{1}{2} \boldsymbol{\varepsilon} \cdot \boldsymbol{\alpha}) \gamma^\mu (1 - \frac{1}{2} \boldsymbol{\varepsilon} \cdot \boldsymbol{\alpha}) \Omega_{\text{op}}^{v_1 \dots v_n}(\mathbf{P}'_{\text{op}}) \psi(R) \\ & \quad - \bar{\psi}(R) \gamma^\mu [\Omega_{\text{op}}^{v_1 \dots v_n}(\mathbf{P}_{\text{op}}), \frac{1}{2} \boldsymbol{\varepsilon} \cdot \boldsymbol{\alpha}] \psi(R), \end{aligned} \quad (\text{A14})$$

(up to first order in  $\boldsymbol{\varepsilon}$ ). Now, since

$$\frac{1}{2} [\boldsymbol{\varepsilon} \cdot \boldsymbol{\alpha}, \gamma^\mu] = \varepsilon_\nu^\mu \gamma^\nu, \quad (\text{A15})$$

with  $\varepsilon_{i0}^i = \varepsilon_{i0}^0 = -\varepsilon^i$  and  $\varepsilon^{ij} = 0$ , one may write this as:

$$\begin{aligned} & \bar{\psi}'(R') \gamma^\mu \Omega_{\text{op}}^{v_1 \dots v_n}(\mathbf{P}'_{\text{op}}) \psi'(R') \\ &= \bar{\psi}(R) (\delta_\nu^\mu + \varepsilon_\nu^\mu) \gamma^\nu \Omega_{\text{op}}^{v_1 \dots v_n}(\mathbf{P}_{\text{op}}) \psi(R) + \bar{\psi}(R) \gamma^\mu \{ \Omega_{\text{op}}^{v_1 \dots v_n}(\mathbf{P}'_{\text{op}}) \\ & \quad - \Omega_{\text{op}}^{v_1 \dots v_n}(\mathbf{P}_{\text{op}}) \} \psi(R) - \bar{\psi}(R) \gamma^\mu [\Omega_{\text{op}}^{v_1 \dots v_n}(\mathbf{P}_{\text{op}}), \frac{1}{2} \boldsymbol{\varepsilon} \cdot \boldsymbol{\alpha}] \psi(R). \end{aligned} \quad (\text{A16})$$

The second term at the right-hand side may be written in a different form by using the relation that follows from (27) and the Dirac equation (1):

$$\Omega_{\text{op}}(\mathbf{P}'_{\text{op}}) - \Omega_{\text{op}}(\mathbf{P}_{\text{op}}) = -c^{-1} \boldsymbol{\varepsilon} \cdot \frac{\partial \Omega_{\text{op}}}{\partial \mathbf{P}_{\text{op}}} H_{\text{op}}, \quad (\text{A17})$$

or, with the commutation rule  $[\mathbf{P}_{\text{op}}, \mathbf{R}] = -i\hbar \mathbf{U}$ ,

$$\Omega_{\text{op}}(\mathbf{P}'_{\text{op}}) - \Omega_{\text{op}}(\mathbf{P}_{\text{op}}) = \frac{i}{\hbar c} [\boldsymbol{\varepsilon} \cdot \mathbf{R} H_{\text{op}}, \Omega_{\text{op}}] - \frac{i}{\hbar c} \boldsymbol{\varepsilon} \cdot \mathbf{R} [H_{\text{op}}, \Omega_{\text{op}}]. \quad (\text{A18})$$

Then the second and third term at the right-hand side of (A16) become together

$$\frac{i}{\hbar} \bar{\psi}(R) \gamma^\mu ([\boldsymbol{\varepsilon} \cdot \mathbf{N}_{\text{op}}, \Omega_{\text{op}}^{v_1 \dots v_n}] - c^{-1} \boldsymbol{\varepsilon} \cdot \mathbf{R} [H_{\text{op}}, \Omega_{\text{op}}^{v_1 \dots v_n}]) \psi(R), \quad (\text{A19})$$

where (34) has been used. From (A16) with this result and the fact that  $\psi$  is

arbitrary (in its dependence on space coordinates) it follows by considering the coefficients of the components of  $\boldsymbol{\varepsilon}$  that the lemma as stated above is proved.

In the main text it was shown that the expectation value of an operator  $\Omega_{\text{op}}$  that depends on the momentum operator and on Dirac matrices changes under pure Lorentz transformations (27) by an amount which is the expectation value of the operator (33):

$$\delta \Omega_{\text{op}} = \frac{i}{\hbar} [\boldsymbol{\varepsilon} \cdot \mathbf{N}_{\text{op}}, \Omega_{\text{op}}]. \quad (\text{A20})$$

On the other hand the expectation value of  $\Omega_{\text{op}}^{v_1 \dots v_n}$  transforms as a tensor if one has

$$\delta \Omega_{\text{op}}^{v_1 \dots v_n} = -\varepsilon_i \sum_{j=1}^n (g^{iv_j} \Omega_{\text{op}}^{v_1 \dots v_{j-1} 0 v_{j+1} \dots v_n} - g^{0v_j} \Omega_{\text{op}}^{v_1 \dots v_{j-1} iv_{j+1} \dots v_n}). \quad (\text{A21})$$

Hence the expectation value of  $\Omega_{\text{op}}$  transforms as a tensor if and only if the right-hand sides of (A20) and (A21) are equal or if

$$[N_{\text{op}}^i, \Omega_{\text{op}}^{v_1 \dots v_n}] = i\hbar \sum_{j=1}^n (g^{iv_j} \Omega_{\text{op}}^{v_1 \dots v_{j-1} 0 v_{j+1} \dots v_n} - g^{0v_j} \Omega_{\text{op}}^{v_1 \dots v_{j-1} iv_{j+1} \dots v_n}). \quad (\text{A22})$$

Comparison of this condition with the lemma condition (A13) shows that the statement that (A12) has tensor character is then and only then equivalent with the statement that the expectation value of  $\Omega_{\text{op}}$  transforms as a four-tensor, if the operator  $\Omega_{\text{op}}$  commutes with the Hamiltonian  $H_{\text{op}}$ , i.e. if  $\Omega_{\text{op}}$  is a conserved quantity. This is the theorem of Felix Klein. (This theorem may alternatively be proved by considering the local conservation law that follows from the commutation of  $\Omega_{\text{op}}$  with the Hamiltonian; see problems 1 and 2.) The treatment given above shows explicitly how local covariance and covariance of expectation values are connected in the general case in which the quantity  $\Omega_{\text{op}}$  is not conserved.

In the following we shall need an extension of the lemma given in (A12–A13) to the case of an operator  $\check{\Omega}_{\text{op}}^v$  which depends also on coordinates and on time in such a way that

$$\begin{aligned} [P_{\text{op}}^i, \check{\Omega}_{\text{op}}^v] &= \frac{\hbar}{i} g^{iv}, \\ \left[ -\frac{\hbar}{ic} \frac{\partial}{\partial t}, \check{\Omega}_{\text{op}}^v \right] &= \frac{\hbar}{i} g^{0v}. \end{aligned} \quad (\text{A23})$$



This means that  $\check{\Omega}_{\text{op}}^{\nu}$  is of the form

$$\check{\Omega}_{\text{op}}^{\nu}(\mathbf{P}_{\text{op}}, R) = R^{\nu} + \Omega_{\text{op}}^{\nu}(\mathbf{P}_{\text{op}}), \quad (\text{A24})$$

where  $\Omega_{\text{op}}^{\nu}(\mathbf{P}_{\text{op}})$  is an operator of the type discussed earlier.

Since the quantity  $\bar{\psi}\gamma^{\mu}R^{\nu}\psi$  transforms as a local tensor density, the statement that  $\bar{\psi}\gamma^{\mu}\check{\Omega}_{\text{op}}^{\nu}\psi$  is a local tensor density under pure Lorentz transformations is equivalent to the statement that  $\bar{\psi}\gamma^{\mu}\Omega_{\text{op}}^{\nu}\psi$  transforms as a tensor. Hence according to the lemma (A12–13) one finds that  $\Omega_{\text{op}}^{\nu}$  fulfils (A13). Now one may check by using (34) that  $R^{\nu}$  satisfies the identity

$$[N_{\text{op}}^i - ctP_{\text{op}}^i, R^{\nu}] = c^{-1}R^i[H_{\text{op}} - i\hbar\partial/\partial t, R^{\nu}] + i\hbar(g^{i\nu}R^0 - g^{0\nu}R^i). \quad (\text{A25})$$

From this relation and (A24) it follows that (A13) is for the present case equivalent with

$$[N_{\text{op}}^i - ctP_{\text{op}}^i, \check{\Omega}_{\text{op}}^{\nu}] = c^{-1}R^i[H_{\text{op}} - i\hbar\partial/\partial t, \check{\Omega}_{\text{op}}^{\nu}] + i\hbar(g^{i\nu}\check{\Omega}_{\text{op}}^0 - g^{0\nu}\check{\Omega}_{\text{op}}^i), \quad (\text{A26})$$

where we used the relations  $[P_{\text{op}}^i, \Omega_{\text{op}}^{\nu}] = 0$  and  $[\partial/\partial t, \Omega_{\text{op}}^{\nu}] = 0$ . In other words we have derived the generalized lemma:

Let  $\check{\Omega}_{\text{op}}^{\nu}$  be a set of operators depending on Dirac matrices, the momentum operator, the coordinates and time in such a way that (A23) is fulfilled. Then the quantity

$$\bar{\psi}(R)\gamma^{\mu}\check{\Omega}_{\text{op}}^{\nu}(\mathbf{P}_{\text{op}}, R)\psi(R) \quad (\text{A27})$$

is – for all solutions  $\psi$  of the Dirac equation for a free particle – a local tensor density under pure Lorentz transformation if and only if the operator relation

$$[N_{\text{op}}^i - ctP_{\text{op}}^i, \check{\Omega}_{\text{op}}^{\nu}] = c^{-1}R^i[H_{\text{op}} - i\hbar\partial/\partial t, \check{\Omega}_{\text{op}}^{\nu}] + i\hbar(g^{i\nu}\check{\Omega}_{\text{op}}^0 - g^{0\nu}\check{\Omega}_{\text{op}}^i) \quad (\text{A28})$$

is valid.

### c. Covariance requirements on the position and spin operator of the free Dirac particle

In the main text we derived the position and spin operator from a number of requirements which it should fulfil. Among them were the conditions (45) and (48–49) which we called the covariance conditions. They were inspired by the analogy with classical reasonings. The imposing of these conditions led to position and spin operators, which (when generalized to the case of a particle in a field) obeyed equations of motion that have the same form as the classical equations of motion for a composite particle.

One may ask oneself how these covariance conditions are related to local covariance and covariance of expectation values, discussed in the preceding subsection in connexion with Klein's theorem. In particular one may wonder whether it is possible to find a position operator  $X_{\text{op}}$  which is the space part of a set of four operators  $\check{X}_{\text{op}}^{\nu}$  ( $\nu = 0, 1, 2, 3$ ) such that  $\bar{\psi}\gamma^{\mu}\check{X}_{\text{op}}^{\nu}\psi$  is a local tensor density. One knows that the space part  $X_{\text{op}}$  should satisfy the property of translation covariance (36). Let us assume moreover that  $X_{\text{op}}$  does not explicitly depend on the time  $t$  and that the time component  $X_{\text{op}}^0$  does not depend explicitly on the coordinates  $\mathbf{R}$  and on the time  $t$  in a way specified by

$$\left[\frac{\partial}{c\partial t}, X_{\text{op}}^0\right] = 1. \quad (\text{A29})$$

Then it follows from the lemma (A27–28) that local covariance of  $\bar{\psi}\gamma^{\mu}\check{X}_{\text{op}}^{\nu}\psi$  leads to four conditions ( $\nu = 0, 1, 2, 3$ )

$$[N_{\text{op}}^i - ctP_{\text{op}}^i, X_{\text{op}}^{\nu}] = c^{-1}R^i[H_{\text{op}} - i\hbar\partial/\partial t, X_{\text{op}}^{\nu}] + i\hbar(g^{i\nu}X_{\text{op}}^0 - g^{0\nu}X_{\text{op}}^i). \quad (\text{A30})$$

Since we are interested in even operators, i.e. operators which contain only even Dirac matrices in the P–FW picture, and since  $\hat{N}_{\text{op}}$  (64),  $\hat{H}_{\text{op}}$  (48) are even but  $\hat{\mathbf{R}}_{\text{op}}$  (61) contains an odd part given in (63), it follows that (A30) cannot be satisfied. Hence four operators  $X_{\text{op}}^{\nu}$  ( $\nu = 0, 1, 2, 3$ ) which would lead to a local four-tensor density  $\bar{\psi}\gamma^{\mu}\check{X}_{\text{op}}^{\nu}\psi$  cannot be found.

Instead one might look for a set of four operators of which the zero component is simply  $ct$  on the argument that in the usual formulation of quantum mechanics the time plays a role which is essentially different from that of the space coordinates. One may try then to impose (A30) for  $\nu = 1, 2, 3$  only, but putting  $X^0$  equal to  $ct$ . If again one assumes that  $X_{\text{op}}$  does not depend explicitly on time, one finds

$$[N_{\text{op}}^i - ctP_{\text{op}}^i, X_{\text{op}}^j] = c^{-1}R^i[H_{\text{op}}, X_{\text{op}}^j] + i\hbar ctg^{ij}. \quad (\text{A31})$$

For the same reasons as given above an even operator  $X_{\text{op}}^i$  satisfying this condition does not exist either.

The condition (A31) is equivalent to the following two conditions, which are half the sum and half the difference of (A31) and its hermitian conjugate

$$0 = [R^i, [H_{\text{op}}, X_{\text{op}}^j]], \quad (\text{A32})$$

$$[N_{\text{op}}^i - ctP_{\text{op}}^i, X_{\text{op}}^j] = \frac{1}{2}c^{-1}\{R^i, [H_{\text{op}}, X_{\text{op}}^j]\} + i\hbar ctg^{ij}. \quad (\text{A33})$$

As seen above no even operator  $X_{\text{op}}^j$  exists satisfying both of these relations. The condition (A32) alone is sufficient already to exclude the existence of a solution, as follows from the general form (59) for the position operator

with (58) and (61). Therefore one may try to impose only (A33), while forgetting about (A32). Using the translation property (36) one may write (A33) as

$$[N_{op}^i, X_{op}^j] = \frac{1}{2}c^{-1}\{R^i, [H_{op}, X_{op}^j]\}. \quad (A34)$$

However by insertion of the general form (59) with (58), (61) and (64) one gets contradictory equations for the form factors  $f_1(E_{op})$  and  $f_2(E_{op})$  so that no even position operator that satisfies (A34) exists.

A different line of approach would consist in requiring the covariance of the expectation value of the position operator instead of local covariance. Then, as follows from (33), we must have

$$[N_{op}^i - ctP_{op}^i, X_{op}^j] = i\hbar ctg^{ij}. \quad (A35)$$

Once more with (59) and (64) inserted one finds a negative result. So this road is blocked as well.

Returning to the condition (A34) one notices that the coordinate  $R^i$  looks like a foreign element since elsewhere in the condition the position  $X_{op}^i$  occurs. So one is led to replace  $R^i$  in (A34) by  $X_{op}^i$ . In that case one gets

$$[N_{op}^i, X_{op}^j] = \frac{1}{2}c^{-1}\{X_{op}^i, [H_{op}, X_{op}^j]\}. \quad (A36)$$

This is precisely the condition of the main text, which has a solution explicitly given there. The considerations given here were only intended to show that various other conceivable requirements do not lead to results.

We now turn to the discussion of the covariance requirements on the spin operator. Since the translation property (37) implies that the spin operator is independent of the coordinates (in the Dirac picture and hence in the P-FW picture), the evenness of the operator in the P-FW picture implies that it is conserved, as follows from (58). This means that the lemma (A12-13) for the spin operator  $s_{op}^{v_1v_2}$  (which will be assumed to be a quantity with two indices in which it is antisymmetric) says that the quantity  $\bar{\psi}\gamma^\mu s_{op}^{v_1v_2}\psi$  is a local covariant tensor if and only if

$$[N_{op}^i, s_{op}^{v_1v_2}] = i\hbar(g^{iv_1}s_{op}^{0v_2} - g^{iv_2}s_{op}^{0v_1} - g^{0v_1}s_{op}^{iv_2} + g^{0v_2}s_{op}^{iv_1}). \quad (A37)$$

From (A22) it then follows that this condition is equivalent with the requirement that the expectation value of the spin operator transforms as a tensor. (This is the application of Klein's theorem to the case of the spin operator.) Written in terms of the operators  $s_{op}^i = \frac{1}{2}\epsilon^{ijk}s_{jk,op}$  and  $t_{op}^i = s_{op}^{i0}$  the condition (A37) reads

$$[N_{op}^i, s_{op}^j] = i\hbar\epsilon^{ijk}t_{k,op}, \quad (A38)$$

$$[N_{op}^i, t_{op}^j] = -i\hbar\epsilon^{ijk}s_{k,op}. \quad (A39)$$

These are the same as (48) and (49), since  $s_{op}$  and  $t_{op}$  are both conserved so that the conditions (48) and (49) are equivalent with both local covariance and covariance of the expectation value of the spin operator. The coinciding of the various possible requirements on the spin operator made the problem to find it essentially simpler than that of the position operator.

d. *Three mutually excluding requirements on the position operator for the free Dirac particle*

In the main text we found that the position operator had non-commuting components. Hence the requirement of commutation of these components is not consistent with the requirements of Lorentz covariance, at least not for an even position operator. One may ask what happens if one would require from the beginning the commutation and forget about covariance. To find the position operator which has this property we insert the general expression (59) for the position operator in the P-FW picture into the commutation rule

$$[\hat{X}_{op}^i, \hat{X}_{op}^j] = 0. \quad (A40)$$

This yields a number of differential equations for the functions  $f_1$  and  $f_2$ . There are three independent solutions. They give rise to the following forms for the position operator in the P-FW picture:

$$\hat{X}_{op} = \mathbf{R}, \quad (A41)$$

$$\hat{X}_{op} = \mathbf{R} - \frac{\hbar c^2}{E_{op}^2 - m^2 c^4} \boldsymbol{\sigma} \wedge \mathbf{P}_{op}, \quad (A42)$$

$$\hat{X}_{op} = \mathbf{R} - \frac{\hbar c^2}{2(E_{op}^2 - m^2 c^4)} (1 \pm \beta) \boldsymbol{\sigma} \wedge \mathbf{P}_{op}. \quad (A43)$$

The second and third solutions have the unwanted property to be singular for zero momentum. If one discards them for that reason, one is left with (A41), which is the position operator of Newton and Wigner<sup>1</sup>. Hence we conclude that if commutation of Cartesian components – as well as a regularity con-

<sup>1</sup> T. D. Newton and E. P. Wigner, Rev. Mod. Phys. **21**(1949)400; K. Bardakci and R. Acharya, N. Cim. **21**(1961)802; P. M. Mathews and A. Sankaranarayanan, Progr. Theor. Phys. **26**(1961)499; **27**(1962)1063; W. Weidlich and A. K. Mitra, N. Cim. **30**(1963)385; U. Schröder, Ann. Physik **14**(1964)91; T. O. Philips, Phys. Rev. **136B**(1964)893; A. Galindo, N. Cim. **37**(1965)413; R. A. Berg, J. Math. Phys. **6**(1965)34; A. Sankaranarayanan and R. H. Good Jr., Phys. Rev. **140B**(1965)509; P. M. Mathews, Phys. Rev. **143**(1966)985; M. Lunn, J. Phys. **A2**(1969)17.

dition – is imposed on the position operator (apart from its translation, rotation, spatial inversion and time reversal properties), one finds the operator of Newton and Wigner. However covariance is then lost.

If one wants to impose both covariance and commutation of the components one is obliged to leave the domain of operators which are even in the P–FW picture. Then one gets afflicted with the interplay of positive and negative energy solutions. If in spite of this one remains interested in the possible forms of operators which fulfil the requirements of covariance and commutation, one may start from the general expression which satisfies the requirements of translation, rotation, spatial inversion and time reversal. In the P–FW picture one has then

$$\hat{X}_{\text{op}} = \mathbf{R} + \{f_1(E_{\text{op}}) + \beta f_2(E_{\text{op}})\} \boldsymbol{\sigma} \wedge \mathbf{P}_{\text{op}} + f_3(E_{\text{op}}) \rho_2 \boldsymbol{\sigma} + f_4(E_{\text{op}}) \rho_2 \mathbf{P}_{\text{op}} \mathbf{P}_{\text{op}} \cdot \boldsymbol{\sigma}. \quad (\text{A44})$$

By imposing the Lorentz covariance condition (60) one finds equations for the  $f_i(E_{\text{op}})$  ( $i = 1, 2, 3, 4$ ). Upon substitution of the solutions into the above expression one obtains two types of possible position operators

$$\hat{X}_{\text{op}} = \mathbf{R} + \frac{\hbar \boldsymbol{\sigma} \wedge \mathbf{P}_{\text{op}}}{2m(E_{\text{op}} + mc^2)} + f_4(E_{\text{op}}) \rho_2 \mathbf{P}_{\text{op}} \mathbf{P}_{\text{op}} \cdot \boldsymbol{\sigma}, \quad (\text{A45})$$

$$\hat{X}_{\text{op}} = \mathbf{R} - \frac{\hbar c^2 \boldsymbol{\sigma} \wedge \mathbf{P}_{\text{op}}}{2E_{\text{op}}(E_{\text{op}} + mc^2)} \pm \frac{\hbar c}{2E_{\text{op}}} \rho_2 \left\{ \boldsymbol{\sigma} - \frac{c^2 \mathbf{P}_{\text{op}} \mathbf{P}_{\text{op}} \cdot \boldsymbol{\sigma}}{E_{\text{op}}(E_{\text{op}} + mc^2)} \right\}. \quad (\text{A46})$$

If one imposes moreover the condition of commutativity of the components of  $\hat{X}_{\text{op}}$ , one finds that the solution (A45) does not fulfil this requirement (for any  $f_4$ ), while (A46) fulfils it as it stands for *both* possible signs. The latter, with the upper sign, is the Dirac position operator in the P–FW picture, as follows from (62) with (63) (keeping in mind that one has  $i\beta\boldsymbol{\alpha} \equiv -\rho_2\boldsymbol{\sigma}$  in the Pauli representation). It is simply  $\mathbf{R}$  in the Dirac picture. The expression (A46) with the minus sign is as good a solution as the Dirac position operator. It reads, in the Dirac picture

$$X_{\text{op}} = \mathbf{R} - \frac{\hbar c^2 \boldsymbol{\sigma} \wedge \mathbf{P}_{\text{op}}}{E_{\text{op}}^2} + \frac{i\hbar mc^3 \beta \boldsymbol{\alpha}}{E_{\text{op}}^2}. \quad (\text{A47})$$

Incidentally it may be remarked that if we impose the evenness instead of the commutativity, one finds as only possibility (A45) with  $f_4 = 0$ , i.e., as it should be, the position operator employed in the main text.

e. *On the uniqueness of the position operator of the free Klein–Gordon particle*

In the main text we found the even part of the position operator from the

requirements of translation, rotation, spatial inversion and time reversal alone. It turned out to satisfy the Lorentz covariance requirement and to possess commuting components. Hence these two latter properties are compatible for even operators in the case of the Klein–Gordon particle.

For purely academic reasons one may still ask which position operators are possible if odd operators are allowed to play a role. Then, from the requirements of translation, rotation, space inversion and time reversal alone, one has for the position operator the form

$$\hat{X}_{\text{op}} = \mathbf{R} + f_1(E_{\text{op}}) \tau_1 \mathbf{P}_{\text{op}}. \quad (\text{A48})$$

This position operator satisfies the Lorentz covariance condition and has also commuting components, for arbitrary function  $f_1$ . Its even part is  $\mathbf{R}$ , which also separately fulfils the requirements of Lorentz covariance and has commuting components.

The possibility of fulfilling simultaneously the requirements of covariance and commutativity for the even part of the position operator makes the treatment of a particle without spin essentially simpler than that of a particle with spin.

### PROBLEMS

1. Show from the Dirac equation (1) that  $j^z \equiv \bar{\psi} \gamma^z \Omega_{op} \psi$  (with  $\Omega_{op}$  independent of the time) is conserved ( $\partial_\alpha j^z = 0$ ) if and only if the operator  $\Omega_{op}$  commutes with the Hamiltonian  $H_{op}$ .

2. Prove F. Klein's theorem in its standard form: if a tensor  $t^{\alpha\beta\dots\mu\nu}$  satisfies a local conservation law  $\partial_\nu t^{\alpha\beta\dots\mu\nu} = 0$  then the quantity  $\int t^{\alpha\beta\dots\mu 0} d\mathbf{R}$  is conserved and is a tensor of the type  $u^{\alpha\beta\dots\mu}$  if the integrand tends to zero at infinity in such a way that surface integrals vanish there.

Hint: since the indices  $\alpha\beta \dots \mu$  appear everywhere in the same way, the theorem is proved if one shows for a vector  $j^z$  with  $\partial_\alpha j^z = 0$  that  $\int j^0 d\mathbf{R}$  is conserved and is a scalar invariant, provided that  $j^0$  vanishes sufficiently quickly at infinity. The proof follows by considering two space-like surfaces  $\sigma$  and  $\hat{\sigma}$ , quantities  $\int j^0 d\mathbf{R} = \int j^z d\sigma_\alpha$  and  $\int j^0 d\mathbf{R}' = \int j^{z'} d\hat{\sigma}'_\alpha = \int j^z d\hat{\sigma}_\alpha$  and by application of Gauss's theorem.

3. Find the unitary transformation (56) by considering the plane wave solutions of the Dirac equation (1) with Hamiltonian (2).

4. Derive the equation of motion that would result if one takes for the position operator of the Dirac particle in an electromagnetic field the operator  $\mathbf{R}$  in the Blount picture. Choose for convenience  $g = 2$  and derive first the Weyl transform of the velocity operator

$$\hat{v}_{op} \equiv \frac{i}{\hbar} [\hat{H}_{op}, \mathbf{R}] \rightleftharpoons \frac{\beta\pi c^2}{E_\pi} + \frac{e\hbar c^3 \beta \mathbf{P} \cdot \mathbf{B}}{2E^3} - \frac{e\hbar c^2 \boldsymbol{\sigma} \wedge \mathbf{E}}{2E(E+mc^2)} + \frac{e\hbar c^4 (2E+mc^2) \mathbf{P}(\mathbf{P} \wedge \boldsymbol{\sigma}) \cdot \mathbf{E}}{2E^3(E+mc^2)^2}.$$

Derive then the equation of motion

$$m \frac{d\hat{\mathbf{v}}_{op}}{dt} \equiv \frac{i}{\hbar} [\hat{H}_{op}, m\hat{\mathbf{v}}_{op}] + m \frac{\partial \hat{\mathbf{v}}_{op}}{\partial t} \rightleftharpoons \gamma^{-2} (\mathbf{U} - \boldsymbol{\beta} \boldsymbol{\beta}) \cdot \left( \gamma e \mathbf{E} + \gamma e \boldsymbol{\beta} \wedge \mathbf{B} + \frac{e\hbar}{2mc} \left[ (\nabla \mathbf{B}) \cdot \boldsymbol{\sigma} + \frac{\gamma}{\gamma+1} (\nabla \mathbf{E}) \cdot (\boldsymbol{\beta} \wedge \boldsymbol{\sigma}) + \gamma^2 (\partial_0 + \boldsymbol{\beta} \cdot \nabla) \left\{ \boldsymbol{\beta} \boldsymbol{\sigma} \cdot \mathbf{B} - \frac{\boldsymbol{\sigma} \wedge \mathbf{E}}{\gamma(\gamma+1)} + \frac{\gamma^2 \boldsymbol{\beta} \boldsymbol{\beta} \cdot (\boldsymbol{\sigma} \wedge \mathbf{E})}{(\gamma+1)^2} \right\} \right] \right),$$

where we limited ourselves to the upper left part of the matrix expression, i.e.  $\beta$  replaced by 1 (necessary for expectation values of the positive energy solutions) and where we used the same abbreviations as given above formula (158). The fields depend on the position  $\mathbf{R}$  and the time  $t$ .

Corresponding to this choice of the position operator one takes now for the spin operator (v. (149)):  $\frac{1}{2} \hbar \boldsymbol{\sigma}$ . Show that the equation for this spin operator becomes (again with  $g = 2$ )

$$\frac{d\boldsymbol{\sigma}}{dt} \equiv \frac{i}{\hbar} [\hat{H}_{op}, \boldsymbol{\sigma}] \rightleftharpoons \frac{e}{mc} \left\{ \gamma^{-1} \boldsymbol{\sigma} \wedge \mathbf{B} - \frac{1}{\gamma+1} \boldsymbol{\sigma} \wedge (\boldsymbol{\beta} \wedge \mathbf{E}) \right\},$$

where again  $\beta$  has been replaced by 1.

The right-hand sides of the equations of motion and spin given above are not covariant. To prove this fact one should show in the first place that the right-hand side of the equation of motion without the factor  $\gamma^{-2} (\mathbf{U} - \boldsymbol{\beta} \boldsymbol{\beta})$  is not the space part of a four-vector. Show this for the terms with field derivatives by writing first the rest frame expression:

$$(\nabla' \mathbf{B}') \cdot \boldsymbol{\sigma}' - \frac{1}{2} \boldsymbol{\sigma}' \wedge \partial'_0 \mathbf{E}'$$

and transforming this with the help of the Lorentz transformation formulae for  $(\partial'_0, \nabla')$  and  $(\mathbf{E}', \mathbf{B}')$ , assuming the transformation character of  $\boldsymbol{\sigma}'$  to have the general form

$$\boldsymbol{\sigma}' = F \boldsymbol{\sigma} + G \boldsymbol{\beta} \boldsymbol{\beta} \cdot \boldsymbol{\sigma}$$

with  $F$  and  $G$  functions of  $|\boldsymbol{\beta}|$  or  $\gamma$ . It turns out then that the difference between this transformed expression and the field derivative terms in the equation of motion is not parallel to the velocity  $\boldsymbol{\beta}$ , so that the non-covariance is then proved.

The non-covariance of the spin equation may be proved along similar lines.

(The covariance of the equations of motion and spin as derived in the main text may be proved with the same technique. Strictly spoken this is not necessary since we started from covariant position and spin operators; moreover the resulting equations have the same form as the manifestly covariant classical equations.)

5. The same questions as those of the preceding problem arise if a still different position operator is adopted, namely one that is connected with the Dirac position operator. Prove first that the operator which is simply  $\mathbf{R}$  in the Dirac picture gets the form (for  $g = 2$ )

$$\hat{\mathbf{R}} \rightleftharpoons \mathbf{R} + \frac{\hbar c^2 \boldsymbol{\pi} \wedge \boldsymbol{\sigma}}{2E_\pi(E_\pi + mc^2)} + \frac{e\hbar^2 c^3 (2E^2 - m^2 c^4) \mathbf{P} \wedge \mathbf{B}}{8E^4(E + mc^2)^2} - \frac{\beta e \hbar^2 c^2}{4E^3} \left( \mathbf{E} - \frac{\mathbf{P} \cdot \mathbf{E}}{E^2} \right) + \hat{\mathbf{R}}_o,$$

in the Blount picture. Here  $\hat{\mathbf{R}}_o$  is the odd part of the transformed Dirac position. Its explicit form is irrelevant if one is interested in the expectation value of positive (or negative) energy solutions: then only the even part of the Dirac position operator comes into play.

Show that the velocity operator corresponding to the even part of the Dirac position is:

$$\hat{v}_{\text{op}} \rightleftharpoons \frac{\beta \pi c^2}{E_\pi} + \frac{e\hbar m c^5 \beta \mathbf{P} \cdot \boldsymbol{\sigma} \cdot \mathbf{B}}{2E^3(E + mc^2)} + \frac{e\hbar c^3 \beta \boldsymbol{\sigma} \cdot \mathbf{P} \cdot \mathbf{B}}{2E^2(E + mc^2)} - \frac{e\hbar m c^4}{2E^3} \boldsymbol{\sigma} \wedge \mathbf{E} - \frac{e\hbar c^4 \mathbf{P} \wedge \mathbf{E} \cdot \boldsymbol{\sigma}}{2E^3(E + mc^2)}.$$

Prove then the equation of motion for this choice of the position operator

$$m \frac{d\hat{v}_{\text{op}}}{dt} \rightleftharpoons \gamma^{-2} (\mathbf{U} - \beta \boldsymbol{\beta}) \cdot \left( \gamma e \mathbf{E} + \gamma e \boldsymbol{\beta} \wedge \mathbf{B} + \frac{e\hbar}{2mc} \left[ (\nabla \mathbf{B}) \cdot \boldsymbol{\sigma} + \frac{\gamma}{\gamma + 1} (\nabla \mathbf{E}) \cdot (\boldsymbol{\beta} \wedge \boldsymbol{\sigma}) + (\partial_0 + \boldsymbol{\beta} \cdot \nabla) \left\{ \frac{\gamma}{\gamma + 1} \boldsymbol{\sigma} \cdot \mathbf{B} + \frac{\gamma^2}{\gamma + 1} \boldsymbol{\beta} \cdot \boldsymbol{\sigma} \cdot \mathbf{B} + \frac{\gamma^3}{\gamma + 1} \boldsymbol{\beta} \boldsymbol{\beta} \cdot \boldsymbol{\sigma} \cdot \mathbf{B} - \gamma^{-1} \boldsymbol{\sigma} \wedge \mathbf{E} - \frac{\gamma}{\gamma + 1} \boldsymbol{\beta} \wedge \mathbf{E} \boldsymbol{\beta} \cdot \boldsymbol{\sigma} - \gamma \boldsymbol{\beta} \boldsymbol{\beta} \cdot (\boldsymbol{\sigma} \wedge \mathbf{E}) \right\} \right] \right).$$

Again  $\beta$  was replaced by 1. The fields in this equation depend on  $\mathbf{R}$  and  $t$ . Introduce now the fields at the position  $\hat{\mathbf{R}}$  and time  $t$ . Introduce moreover the even part  $\frac{1}{2}\hbar\hat{\boldsymbol{\sigma}}_{e,\text{op}}$  of the spin operator that corresponds to the Dirac position operator, i.e. the operator which is  $\frac{1}{2}\hbar\boldsymbol{\sigma}$  in the Dirac picture. Prove first that the Blount picture expression of this spin operator is, up to terms without potentials and fields (needed only for the equation of motion):

$$\hat{\boldsymbol{\sigma}}_{\text{op}} \rightleftharpoons \hat{\boldsymbol{\sigma}}_e + \hat{\boldsymbol{\sigma}}_o$$

with the even part

$$\hat{\boldsymbol{\sigma}}_e = \boldsymbol{\sigma} - \frac{c^2 \mathbf{P} \wedge (\boldsymbol{\sigma} \wedge \mathbf{P})}{E(E + mc^2)} = \boldsymbol{\sigma} - \frac{\gamma \boldsymbol{\beta} \wedge (\boldsymbol{\sigma} \wedge \boldsymbol{\beta})}{\gamma + 1}$$

(which might be written as  $\hat{\boldsymbol{\sigma}}_e = \gamma^{-1} \boldsymbol{\Omega}^{-1} \cdot \boldsymbol{\sigma}$ ) and  $\hat{\boldsymbol{\sigma}}_o$  the odd part which need

not be specified. Show that the equation of motion then gets the form

$$m \frac{d\hat{\boldsymbol{\sigma}}_{\text{op}}}{dt} \rightleftharpoons \gamma^{-2} (\mathbf{U} - \beta \boldsymbol{\beta}) \cdot \left( \gamma e \mathbf{E} + \gamma e \boldsymbol{\beta} \wedge \mathbf{B} + \frac{e\hbar}{2mc} [(\nabla \mathbf{B}) \cdot \hat{\boldsymbol{\sigma}}_e + \gamma^2 (\partial_0 + \boldsymbol{\beta} \cdot \nabla) \{ \boldsymbol{\beta} \hat{\boldsymbol{\sigma}}_e \cdot \mathbf{B} - \gamma^{-2} \hat{\boldsymbol{\sigma}}_e \wedge \mathbf{E} - \boldsymbol{\beta} \boldsymbol{\beta} \cdot (\hat{\boldsymbol{\sigma}}_e \wedge \mathbf{E}) \}] \right).$$

To derive the spin equation show first that the even part of the spin operator which is simply  $\frac{1}{2}\hbar\boldsymbol{\sigma}$  in the Dirac picture, reads (up to terms with potentials) in the Blount picture (again  $g = 2$ ):

$$\hat{\boldsymbol{\sigma}}_e = \boldsymbol{\sigma} - \frac{c^2 \boldsymbol{\pi} \wedge (\boldsymbol{\sigma} \wedge \boldsymbol{\pi})}{E_\pi(E_\pi + mc^2)}.$$

Derive then the equation of motion for this spin operator:

$$\frac{d\hat{\boldsymbol{\sigma}}_{e,\text{op}}}{dt} \rightleftharpoons \frac{e}{mc} \gamma^{-1} \{ \hat{\boldsymbol{\sigma}}_e \wedge \mathbf{B} + (\hat{\boldsymbol{\sigma}}_e \wedge \mathbf{E}) \wedge \boldsymbol{\beta} \}.$$

Just as in the preceding problem one may prove the non-covariance of the right-hand sides of the equations of motion and spin.

6. Prove from (158) that one has for the inner product of  $\hat{\boldsymbol{\sigma}}_{\text{op}}$  and  $m d\hat{\boldsymbol{\sigma}}_{\text{op}}/dt$  the equation:

$$\frac{1}{2} m \left\{ \hat{\boldsymbol{\sigma}}_{\text{op}} \cdot \frac{d\hat{\boldsymbol{\sigma}}_{\text{op}}}{dt} \right\} \rightleftharpoons \gamma^{-4} \left[ c\gamma e \boldsymbol{\beta} \cdot \mathbf{E}(\hat{\mathbf{X}}, t) + \frac{ge}{2m} \{ \boldsymbol{\beta} \cdot (\nabla \mathbf{B}) \cdot \hat{\boldsymbol{\sigma}} + \boldsymbol{\beta} \cdot (\nabla \mathbf{E}) \cdot (\boldsymbol{\beta} \wedge \hat{\boldsymbol{\sigma}}) + \gamma^2 \boldsymbol{\beta}^2 (\partial_0 + \boldsymbol{\beta} \cdot \nabla) \hat{\boldsymbol{\sigma}} \cdot (\mathbf{B} - \boldsymbol{\beta} \wedge \mathbf{E}) \} - \frac{(g-2)e}{2m} \gamma^2 (\partial_0 + \boldsymbol{\beta} \cdot \nabla) (\boldsymbol{\beta} \wedge \hat{\boldsymbol{\sigma}}) \cdot (\mathbf{E} + \boldsymbol{\beta} \wedge \mathbf{B}) \right].$$

Compare this result with that of problem 10 of chapter IV.