V Relativistic quantum mechanics

- The free Schrödinger equation

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

is based on the non-relativistic energy-momentum relation

$$E = \frac{\vec{p}^{\,2}}{2m} .$$

- This is a limiting case of the relativistic relation

$$E = \sqrt{\vec{p}^{\,2} c^2 + m^2 c^4} .$$

- In this chapter we will discuss how one can construct a „relativistic Schrödinger equation", based on this more general expression.
- This connection between quantum theory and special relativity leads to new phenomena and also requires new interpretations, e.g. it shows that a many-particle theory is ultimately necessary in order to arrive at a consistent picture.

VI The Klein-Gordon equation

- The free Schrödinger equation is obtained by making the substitutions

$$E \rightarrow i\hbar \frac{\partial}{\partial t}$$

$$\vec{p} \rightarrow \frac{\hbar}{i} \nabla$$

in the energy momentum relation $E = \frac{p^2}{2m}$.

- Attempting this for the relativistic expression leads to

$$i\hbar \frac{\partial}{\partial t} \psi(\vec{x},t) = \sqrt{-\hbar^2 c^2 \Delta + m^2 c^2}\, \psi(\vec{x},t)$$

$$= mc^2 \sqrt{1 - \lambda\!\!\!^{-2} \Delta}\, \psi(\vec{x},t) .$$

(reduced) Compton wavelength $\lambda\!\!\!^{-} = \frac{\hbar}{mc}$

- This equation has problems, which stem from the square root, whose series expansion leads to arbitrarily high powers of Δ.
- This neither leads to a simple theory, nor does it lead to a local and causal description of the physics (wave packets propagate arbitrarily fast).

- On the other hand, this approach cannot be entirely incorrect, since the expansion

$$\sqrt{\vec{p}^2c^2+m^2c^4} \approx mc^2 + \frac{\vec{p}^2}{2m} - \frac{\vec{p}^4}{8m^3c^2}$$

leads to relativistic corrections of the bound state energies of hydrogen (fine structure), which are measurable and rather accurately described.

- To get rid of the square root we revise our starting point and use the squared energy-momentum relationship:

$$E^2 = \vec{p}^2c^2 + m^2c^4 .$$

- This results in the Klein-Gordon equation, which has the form of a wave equation:

$$\left(\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \Delta + \left(\frac{mc}{\hbar}\right)^2\right)\psi(\vec{x},t) = 0 .$$

- Note, that this equation is of second order in the time variable, i.e. we would need two initial values, $\psi(\vec{x},0)$ and $\frac{\partial}{\partial t}\psi(\vec{x},t)\big|_{t=0}$, to propagate it.
- Just like the Schrödinger equation, the Klein-Gordon equation has plane wave solutions:

$$\psi(\vec{x},t) = e^{\frac{i}{\hbar}(\vec{p}\cdot\vec{x} - E(p)t)}$$

- In order to see which energie $E(p)$ are permissible, we insert the plane waves into the equation.

$$\hookrightarrow \; -\frac{E^2}{c^2\hbar^2} + \frac{\vec{p}^{\,2}}{\hbar^2} + \left(\frac{mc}{\hbar}\right)^2 = 0$$

$$\hookrightarrow \; E^2 = \vec{p}^{\,2}c^2 + m^2c^4 \;\rightarrow\; E = \pm\sqrt{\vec{p}^{\,2}c^2 + m^2c^4}$$

- For given $\vec{p}$ the plane waves thus have the form $\psi(\vec{x},t) = e^{\frac{i}{\hbar}\left(\vec{p}\cdot\vec{x} \pm \sqrt{\vec{p}^{\,2}c^2 + m^2c^4}\, t\right)}$.
- Apparently, there are solutions with negative energy and moreover the energy is not bounded from below.
- This is problematic, because it is unclear what the lowest energy state (ground state) of a free particle would be.
- Moreover, the appearance of negative energies affects the interpretation of the wave function as probability amplitude, as we show now:
- For the Schrödinger equation there exists the continuity equation

$$\frac{\partial \rho}{\partial t} + \nabla\cdot\vec{j} = 0, \text{ with } \rho = \psi^*\psi \text{ and } \vec{j} = \frac{\hbar}{2mi}\left(\psi^*\nabla\psi - (\nabla\psi^*)\psi\right).$$

- Here ρ is the positive definite probability density and $\vec{j}$ the probability current.
- To obtain the continuity equation that corresponds to the Klein-Gordon equation we calculate

$$\underbrace{\psi^*\left(\frac{1}{c^2}\frac{\partial^2}{\partial t^2}-\Delta+\left(\frac{mc}{\hbar}\right)^2\right)\psi}_{\text{Klein-Gordon equation}}-\underbrace{\psi\left(\frac{1}{c^2}\frac{\partial^2}{\partial t^2}-\Delta+\left(\frac{mc}{\hbar}\right)^2\right)\psi^*}_{\text{conjugate Klein-Gordon equation}}=0$$

$$\hookrightarrow \frac{1}{c^2}\left(\psi^*\frac{\partial^2}{\partial t^2}\psi-\psi\frac{\partial^2}{\partial t^2}\psi^*\right)-\left(\psi^*\Delta\psi-\psi\Delta\psi^*\right)=0$$

$$\hookrightarrow \frac{1}{c^2}\frac{\partial}{\partial t}\left(\psi^*\frac{\partial}{\partial t}\psi-\psi\frac{\partial}{\partial t}\psi^*\right)-\nabla\cdot\left(\psi^*\nabla\psi-\psi\nabla\psi^*\right)=0$$

- Here we can identify the following qualities:

$$\vec{j}=\frac{\hbar}{2mi}\left(\psi^*\nabla\psi-\psi\nabla\psi^*\right)$$ ... probability current

$$\rho=\frac{i\hbar}{2mc^2}\left(\psi^*\frac{\partial\psi}{\partial t}-\psi\frac{\partial\psi^*}{\partial t}\right)$$ ... „probability density"

- Unlike for the Schrödinger equation, ρ contains a derivative of the wave function.
- Inserting plane waves, one finds that ρ is not positive definite:

$$\hookrightarrow \rho=\frac{i\hbar}{2mc^2}\left(-\frac{iE}{\hbar}-\frac{iE}{\hbar}\right)=\frac{E}{mc^2}$$ ⚠ E can be negative!

- Interestingly, Schrödinger first attempted to formulate a relativistic wave equation, but then discarded his attempts due to such problem.
- The issue is „fixed" within the framework of quantum field theory.
- Here one can use the Klein-Gordon equation for describing spin-less particles and their anti particles.
- The negative „probability density" is cured by multiplying it with the particle charge and interpreting it as charge density.

V. 2 The Dirac equation

- Dirac was wandering whether there exists an equation which is relativistically covariant (like the wave equation), but which contains only a first derivative with respect to time.
- The latter would fix the issue with the negative probability density.
- He constructed indeed an equation of the form

$$i\hbar \frac{\partial}{\partial t} \psi = H_{Dirac} \psi ,$$

with a Hamiltonian H_{Dirac} that is linear in the momentum operator $\vec{p}$.

- This equation also obeys the relativistic energy - momentum relation, reduces to the Schrödinger equation in the nonrelativistic limit and also introduces the spin in a natural way.
- To arrive at his equation, Dirac made the ansatz

$$H_{Dirac} = c\vec{\alpha}\cdot\vec{p} + \beta mc^2 = \frac{c\hbar}{i}\vec{\alpha}\cdot\nabla + \beta mc^2,$$

with α^j and β being constant „coefficients".

- The Dirac equation then reads

$$i\hbar\frac{\partial\psi(\vec{x},t)}{\partial t} = \left(\frac{c\hbar}{i}\vec{\alpha}\cdot\nabla + \beta mc^2\right)\psi(\vec{x},t) = \left(\frac{c\hbar}{i}\alpha^j\partial_j + \beta mc^2\right)\psi(\vec{x},t),$$

where we used the short hand notation $\partial_j = \frac{\partial}{\partial x_j}$ and also the Einstein convention, i.e. the implied summation over indices that appear twice.

- To determine the coefficients, we „square" the equation:

$$-\hbar^2\frac{\partial^2\psi}{\partial t^2} = \left(\frac{c\hbar}{i}\alpha^j\partial_j + \beta mc^2\right)\left(\frac{c\hbar}{i}\alpha^k\partial_k + \beta mc^2\right)\psi$$

$$= -\hbar c^2\frac{1}{2}\left(\alpha^j\partial_j\alpha^k\partial_k + \alpha^k\partial_k\alpha^j\partial_j\right)\psi - i\hbar mc^3\left(\alpha^j\beta + \beta\alpha^j\right)\partial_j\psi$$

$$+ \beta^2 m^2 c^4\psi$$

- Imposing the relativistic energy momentum relation we have to require that this equation becomes the Klein-Gordon equation

$$-\hbar^2 \frac{\partial^2 \psi}{\partial t^2} = -\hbar^2 c^2 \Delta \psi + m^2 c^4 \psi .$$

- Comparing the two equations, we find that the coefficients have to obey

$$\alpha^j \alpha^k + \alpha^k \alpha^j = 2\delta^{jk}$$
$$\alpha^j \beta + \beta \alpha^j = 0$$
$$\beta^2 = 1$$

- These conditions cannot we satisfied using complex numbers, but instead one has to choose α^k and β to be matrices.
- These matrices have to be hermitean (since H_{Dirac} has to be hermitean).
- The last equation shows that β has to be invertible, with $\beta^{-1} = \beta$.
- Making use of this fact, allows to rewrite the second equation as $\alpha^j = -\beta \alpha^j \beta$, and thus

$$\mathrm{Tr}(\alpha^j) = \mathrm{Tr}(-\beta\alpha^j\beta) = \mathrm{Tr}(-\beta^2\alpha^j) = -\mathrm{Tr}(\alpha_j)$$

$\hookrightarrow$ $\mathrm{Tr}(\alpha^j) = 0$.

- Using $(\alpha^j)^2 = 1$, which follows from the first equation, one finds $\mathrm{Tr}(\beta) = 0$.

- The lowest dimension for which matrices with this property can be constructed is 4.
- There are different possibilities to choose them, with the standard choice being

$$\alpha^j = \begin{pmatrix} 0 & \sigma^j \\ \sigma^j & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & -\mathbb{1} \end{pmatrix}$$

σ^j: 2×2 Pauli matrices; $\mathbb{1}$: 2×2 identity matrix

$$\sigma^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

- Given the fact that H_{Dirac} is a 4×4 matrix, the wave function acquires four components:

$$\psi(\vec{x},t) = \begin{pmatrix} \psi_1(\vec{x},t) \\ \psi_2(\vec{x},t) \\ \psi_3(\vec{x},t) \\ \psi_4(\vec{x},t) \end{pmatrix}$$

- This object is called a <u>spinor</u>. (Note, that this is not a vector, as it transformed differently.)
- In summary, the free Dirac equation reads

$$i\hbar \frac{\partial \psi(\vec{x},t)}{\partial t} = \left(\frac{c\hbar}{i} \vec{\alpha} \cdot \nabla + \beta m c^2 \right) \psi(\vec{x},t), \quad \text{or}$$

$$i\hbar \frac{\partial}{\partial t} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix} = \begin{pmatrix} mc^2\psi_1 - ic\hbar\left(\frac{\partial \psi_4}{\partial x} - i\frac{\partial \psi_4}{\partial y}\right) - ic\hbar \frac{\partial \psi_3}{\partial z} \\ mc^2\psi_2 - ic\hbar\left(\frac{\partial \psi_3}{\partial x} + i\frac{\partial \psi_3}{\partial y}\right) + ic\hbar \frac{\partial \psi_4}{\partial z} \\ -mc^2\psi_3 - ic\hbar\left(\frac{\partial \psi_2}{\partial x} - i\frac{\partial \psi_2}{\partial y}\right) - ic\hbar \frac{\partial \psi_1}{\partial z} \\ -mc^2\psi_4 - ic\hbar\left(\frac{\partial \psi_1}{\partial x} + i\frac{\partial \psi_1}{\partial y}\right) + ic\hbar \frac{\partial \psi_2}{\partial z} \end{pmatrix}.$$

- To construct the continuity equation, we define the adjoint spinor

$$\psi^+ = (\psi_1^*, \psi_2^*, \psi_3^*, \psi_4^*)$$

and the adjoint Dirac equation

$$-i\hbar \frac{\partial \psi^+}{\partial t} = -\frac{c\hbar}{i}(\nabla\psi^+)\cdot\vec{\alpha}^+ + \psi^+\beta^+ mc^2 = -\frac{c\hbar}{i}(\vec{\nabla}\psi^+)\cdot\vec{\alpha} + \psi^+\beta mc^2$$

- We now multiply the Dirac equation from the left with ψ^+ and the adjoint equation from the right with ψ.
- Subtracting the two expressions yields

$$\psi^+ i\hbar\frac{\partial\psi}{\partial t} - \left(-i\hbar\frac{\partial\psi^+}{\partial t}\right)\psi = \frac{c\hbar}{i}\psi^+\vec{\alpha}\cdot\nabla\psi + mc^2\psi^+\beta\psi$$
$$- \left(-\frac{c\hbar}{i}(\nabla\psi^+)\cdot\vec{\alpha}\psi + mc^2\psi^+\beta\psi\right),$$

which can be written as

$$i\hbar\frac{\partial}{\partial t}(\psi^+\psi) = \frac{c\hbar}{i}\vec{\nabla}(\psi^+\vec{\alpha}\psi).$$

- This allows to identify the probability current

$$\vec{j} = c\,\psi^+\vec{\alpha}\psi$$

and the probability density

$$\rho = \psi^+\psi = \sum_{i=1}^{4}|\psi_i|^2,$$

which is clearly positive definite.

V.3 Theory of relativity basics

- We already mentioned that the Dirac equation is compatible with the principle of relativity, i.e. the Dirac equation is <u>covariant</u>.

- To understand and analyse what this means precisely, we revisit in the following the basics of the theory of relativity.

- Einstein's postulates:

  i) The laws of physics acquire the same form in any inertial frame of reference, i.e., it is not possible to detect experimentally absolute motion.

  ii) The speed of light is the same in any intertial frame of reference, i.e. it is a universal constant, independently of the reference frame.

- From the second postulate follows, that time cannot be absolute, but that it is connected with space such that when changing between inertial frames of reference also the notion of time must change.

- Such change between reference frames is conducted through a Lorentz transformation, and the invariance of physical laws under this transformation is the central claim of the theory of relativity.
- A space-time point is determined by a four-vector

contravariant four-vector (index at top)

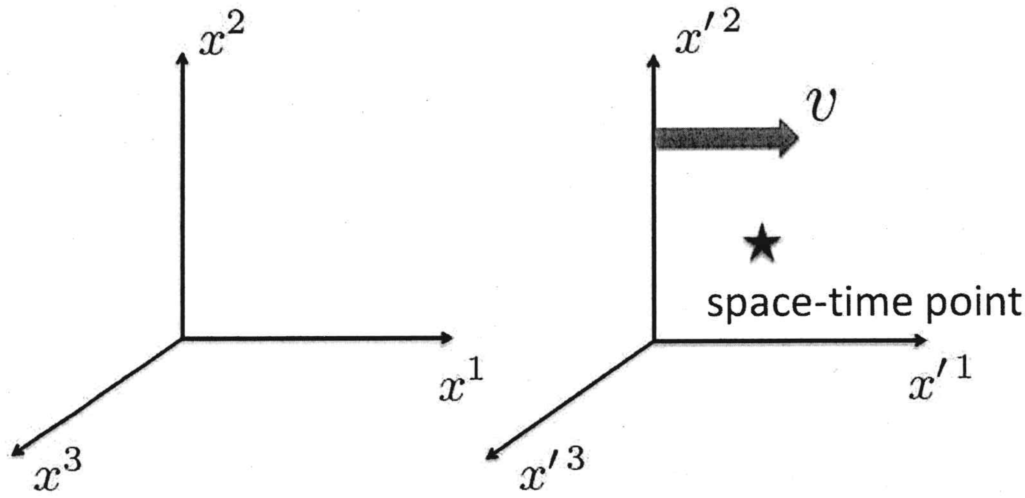
$$x \equiv (ct, \vec{x}) = (ct, x, y, z) \equiv (x^0, x^1, x^2, x^3) \equiv (x^\mu)$$

- We consider now two intertial frames of reference, IS and IS', which at $t=0$ have the same origin $\vec{x}=0$.
- The system IS' moves with constant velocity v into the positive x'-direction.
- These two inertial frames of reference are linked by the <u>Lorentz-boost</u>

$$\underbrace{\begin{matrix} x'^0 \\ x'^1 \\ x'^2 \\ x'^3 \end{matrix}}_{\text{coordinates in IS'}} \begin{matrix} = \\ = \\ = \\ = \end{matrix} \underbrace{\begin{matrix} \gamma x^0 - \beta\gamma x^1 \\ -\beta\gamma x^0 + \gamma x^1 \\ x^2 \\ x^3 \end{matrix}}_{\text{coordinates in IS}},$$

where $\beta = \frac{v}{c}$ and $\gamma = \frac{1}{\sqrt{1-\beta^2}}$.

Intertial frames of reference



Skript zur Vorlesung
Fortgeschrittene Quantentheorie
(Quantenmechanik II)

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- One can show that

$$(x'^0)^2 - (\vec{x}')^2 = (x^0)^2 - \vec{x}^2,$$

which is a consequence of the invariance of the speed of light (the wave front of a light pulse starting from the centre of an inertial frame of reference moves at the speed of light in any frame).

- There are other transformations that leave $(ct)^2 - \vec{x}^2$ invariant, such as rotations of two inertial frames of reference with respect to one another ($\vec{x}$ is invariant under rotations).
- Other examples are parity, $\vec{x} \to -\vec{x}$, and time reversal, $t \to -t$.

- We continue by introducing the so-called covariant four-vector

$$(x_\mu) = (x_0, x_1, x_2, x_3) \equiv (ct, -\vec{x}).$$

- With its help we can write

$$(ct)^2 - \vec{x}^2 = \sum_{\mu=0,1,2,3} x^\mu x_\mu \equiv \underbrace{x^\mu x_\mu}_{\text{Summation convention}} \equiv x \cdot x .$$

- For two different space-time points x and y one has

$$x^0 y^0 - \vec{x} \cdot \vec{y} = x^\mu y_\mu \equiv x \cdot y$$

- It turns out to be useful to introduce the <u>metric tensor</u> $g_{\mu\nu}$, which is defined via

$$x_\mu = \sum_\nu g_{\mu\nu} x^\nu \equiv g_{\mu\nu} x^\nu .$$

$\uparrow$ covariant four-vector

$\uparrow$ contravariant four-vector

- Likewise, one has

$$x^\mu = g^{\mu\nu} x_\nu .$$

- The matrix representation of the metric tensor is

$$(g_{\mu\nu}) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} = (g^{\mu\nu}),$$

with which one finds

$$x \cdot y = x^\mu y_\mu = x^\mu g_{\mu\nu} y^\nu = x_\nu y^\nu = x_\nu g^{\nu\mu} y_\mu .$$

- The quantity $x \cdot y$ is the scalar product (or inner product) of four-vectors.
- It does not change under a Lorentz-transformation, which can be written as

$$x'^\mu = \Lambda^\mu{}_\nu x^\nu \quad \text{or} \quad x' = \Lambda x .$$

- The transformation matrix Λ for the Lorentz-boost on p. 186 reads

$$(\Lambda^\mu{}_\nu) = \begin{pmatrix} \gamma & -\beta\gamma & 0 & 0 \\ -\beta\gamma & \gamma & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad \text{with } \beta = \frac{v}{c},\ \gamma = \frac{1}{\sqrt{1-\beta^2}}.$$

- For a rotation around the x^3-axis by an angle θ, one finds

$$(\Lambda^\mu{}_\nu) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos\theta & \sin\theta & 0 \\ 0 & -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

- We now investigate how certain quantities behave under a Lorentz transformation.
- As mentioned before, the scalar product of two four-vectors, e.g. $x \cdot y$, is the same in any coordinate system.
- Such quantity is called <u>(Lorentz-) scalar</u>, e.g. mass, charge, speed of light and scalar products of four-vectors.
- Any quantity, that transforms like x^μ, is a <u>contravariant four-vector</u>, e.g. $(v^\mu) = (v^0, v^1, v^2, v^3)$ with $v'^\mu = \Lambda^\mu{}_\nu v^\nu$.

- Covariant four-vectors transform according to

$$V'_\mu = \Lambda_\mu{}^\nu V_\nu .$$

- <u>Examples:</u>

i) Four-momentum:

relativistic energy

$$(p^\mu) = \begin{pmatrix} p^0 \\ \vec{p} \end{pmatrix} = \begin{pmatrix} E/c \\ \vec{p} \end{pmatrix}$$

- The quantity $p^\mu p_\mu$ is a scalar:

$$p^\mu p_\mu = \frac{E^2}{c^2} - \vec{p}^{\,2} = mc^2, \text{ i.e.}$$

$$E = \sqrt{\vec{p}c^2 + m^2c^4}$$

ii) Four-gradient:

$$\left(\frac{\partial}{\partial x^\mu}\right) = \left(\frac{\partial}{\partial x^0}, \frac{\partial}{\partial x^1}, \frac{\partial}{\partial x^2}, \frac{\partial}{\partial x^3}\right) \equiv \left(\frac{1}{c}\frac{\partial}{\partial t}, \nabla\right)$$

- Using the chain rule one finds that this quantity transforms like a covariant vector and thus one writes $\frac{\partial}{\partial x^\mu} \equiv \partial_\mu$.

- The corresponding contravariant four-vector is

$$(\partial^\mu) = \left(\frac{\partial}{\partial x_\mu}\right) \equiv \left(\frac{1}{c}\frac{\partial}{\partial t}, -\nabla\right).$$

- With the four-gradient we can calculate the four-divergence, e.g. of the four-vector $(j^\mu) = (j^0, \vec{j})$.

$$\partial_\mu j^\mu = \frac{1}{c}\frac{\partial}{\partial t} j^0 + \vec{\nabla}\cdot\vec{j},$$

which is a Lorentz-invariant quantity.

- We also find that the d'Alembert-operator

$$\partial_\mu \partial^\mu = \frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \Delta^2$$

is a Lorentz-scalar.

iii) Four-vectorpotential:

$$(A^\mu) = \begin{pmatrix} A^0 \\ \vec{A} \end{pmatrix} = \begin{pmatrix} \frac{1}{c}\phi \\ \vec{A} \end{pmatrix}$$

scalar potential

vector potential

V.4 Covariant form of the Dirac equation

- In order to investigate the relativistic covariance of the Dirac-equation we change its representation, by introducing the matrices

$$\gamma^0 \equiv \beta \quad \text{and} \quad \gamma^j \equiv \beta\alpha^j .$$

- Multiplying the Dirac equation from the left with $\beta = \gamma^0$, dividing by c and rearranging it, leads to

$$\left(i\hbar\gamma^0 \frac{1}{c}\frac{\partial}{\partial t} - \frac{\hbar}{i}\vec{\gamma}\cdot\nabla - mc\right)\psi(x) = 0 .$$

four-vector argument

- When introducing $(\gamma^\mu) = (\gamma^0, \vec{\gamma})$ and the notation

$$\underbrace{\not{a}}_{\text{"a-slash"}} \equiv \gamma^\mu \overbrace{a_\mu}^{\text{four-vector}} = \gamma_\mu a^\mu = \gamma^0 a^0 - \vec{\gamma}\cdot\vec{a}\,,$$

we can write the Dirac equation even more compactly,

$$(i\hbar \not{\partial} - mc)\,\psi(x) = 0\,,$$

or, with the four-momentum operator

$$(\hat{\not{p}} - mc) = 0 \qquad , \qquad (\hat{p}^\mu) = i\hbar\,(\partial^\mu)\,.$$

- The matrices, that we introduced at the beginning of this section are the so-called <u>Dirac-matrices or Gamma-matrices.</u>
- Their standard representation is

$$\gamma^0 = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & -\mathbb{1} \end{pmatrix} \quad , \quad \gamma^j = \begin{pmatrix} 0 & \sigma^j \\ -\sigma^j & 0 \end{pmatrix}.$$

- They obey the anti-commutator

$$\{\gamma^\mu, \gamma^\nu\} = 2g^{\mu\nu}\,,$$

from which follows that

$$(\gamma^0)^2 = -(\gamma^j)^2 = 1\,.$$

- A useful relation is

$$(\gamma^\mu)^\dagger = \gamma^0 \gamma^\mu \gamma^0 \iff \begin{cases} (\gamma^0)^\dagger = \gamma^0 \\ (\gamma^j)^\dagger = -\gamma^j \end{cases}$$

- Finally, we construct the four-current density for the Dirac-spinor

$$j^\mu = (c\varrho, \vec{j}).$$

$$\underset{\text{probability density}}{\uparrow} \qquad \underset{\text{current density}}{\nwarrow}$$

- Using $(\gamma^0)^2 = \mathbb{1}$, one finds

$$c\varrho = c\psi^+\psi = c\psi^+\gamma^0\gamma^0\psi = c\bar{\psi}\gamma^0\psi,$$

where $\bar{\psi} \equiv \psi^+\gamma^0$ is the adjoint Dirac-spinor.

- Furthermore,

$$j^k = c\,\psi^+\alpha^k\psi = c\psi^+\gamma^0\underbrace{\gamma^0\alpha^k}_{=\beta\alpha^k=\gamma^k}\psi = c\bar{\psi}\gamma^k\psi.$$

- The four-current density is thus

$$j^\mu = c\bar{\psi}\gamma^\mu\psi,$$

and it obeys the continuity equation

$$\partial_\mu j^\mu = 0.$$

V.5 Solution of the free Dirac equation

- We make the plane wave ansatz

$$\psi(x) = u(p)\,e^{-\frac{i}{\hbar}p\cdot x} = u(p)\,e^{-\frac{i}{\hbar}(Et-\vec{p}\cdot\vec{x})},$$

with the spinor $u(p)$ that has as its argument the four-momentum

$p = (\frac{E}{c}, \vec{p})$.

- Inserting the ansatz into the Dirac-equation yields
$$(\overbrace{\gamma^\mu p_\mu}^{\not{p}} - mc)\, u(p) = 0 .$$
- This set of equations has a solution, when the determinant
$$\det(\not{p} - mc) = \det \begin{pmatrix} \frac{E}{c} - mc & 0 & -p^z & -p^x + ip^y \\ 0 & \frac{E}{c} - mc & -p^x - ip^y & p^z \\ p^z & p^x - ip^y & -\frac{E}{c} - mc & 0 \\ p^x + ip^y & -p^z & 0 & -\frac{E}{c} - mc \end{pmatrix}$$
$$= \frac{1}{c^4}\left(E^2 - (\vec{p}^{\,2} c + m^2 c^4)\right)^2$$
vanishes.
- This happens when
$$E = \pm\sqrt{\vec{p}^{\,2} c^2 + m^2 c^4} \equiv E^\pm .$$
- Apparently, there are also solutions with negative energy.
- In principle, one can now solve the set of equations for given $E^\pm$ in order to obtain the associated spinor $u(p)$.
- We pursue a simpler way, which starts from the solution in the rest frame, $\vec{p} = 0$, where the Dirac equation becomes
$$\begin{pmatrix} E - mc^2 & 0 & 0 & 0 \\ 0 & E - mc^2 & 0 & 0 \\ 0 & 0 & -E - mc^2 & 0 \\ 0 & 0 & 0 & -E - mc^2 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{pmatrix} = 0 .$$

- This has the four linearly independent solutions:

$$E = mc^2 : \begin{pmatrix}1\\0\\0\\0\end{pmatrix}, \begin{pmatrix}0\\1\\0\\0\end{pmatrix} \quad ; \quad E = -mc^2 : \begin{pmatrix}0\\0\\1\\0\end{pmatrix}, \begin{pmatrix}0\\0\\0\\1\end{pmatrix} .$$

- We consider now the expression

$$(\not{p} - mc)(\not{p} + mc) = \not{p}\not{p} - m^2c^2 = p_\mu p_\nu \gamma^\mu \gamma^\nu - m^2c^2$$
$$= p_\mu p_\nu \frac{1}{2}\{\gamma^\mu, \gamma^\nu\} - m^2c^2$$
$$= p^2 - m^2c^2$$
$$= \frac{E^2}{c^2} - \vec{p}^{\,2} - m^2c^2 = 0 .$$

- This means that for any given spinor ω, the spinor $(\not{p} + mc)\omega$ is a solution of the Dirac equation.

- Using the matrix representation of $\not{p} + mc$ with energy E^+ and applying it to the spinors $\begin{pmatrix}1\\0\\0\\0\end{pmatrix}$ and $\begin{pmatrix}0\\1\\0\\0\end{pmatrix}$ yields the positive energy solutions, which allow to construct the normalised wave functions

$$\psi^{(1)}(x) = e^{-\frac{i}{\hbar} p(E^+)\cdot x}\, u^{(1)}(p(E^+)) = \underbrace{\frac{e^{-\frac{i}{\hbar}(E^+ t - \vec{p}\cdot\vec{x})}}{\sqrt{2mc^2(E^+ + mc^2)}}}_{\text{normalisation constant}} \underbrace{\begin{pmatrix} E^+ + mc^2 \\ 0 \\ c p^z \\ c(p^x + i p^y) \end{pmatrix}}_{u^{(1)}(p(E^+))}$$

and

$$\psi^{(2)}(x) = \frac{e^{-\frac{i}{\hbar}(E^+ t - \vec{p}\cdot\vec{x})}}{\sqrt{2mc^2(E^+ + mc^2)}} \begin{pmatrix} 0 \\ E^+ + mc^2 \\ c(p^x - i p^y) \\ -c p^z \end{pmatrix} .$$

- For constructing the wave functions associated with the rest frame spinors $\begin{pmatrix}0\\0\\1\\0\end{pmatrix}$ and $\begin{pmatrix}0\\0\\0\\1\end{pmatrix}$ we use $E = E^-$ (we cannot use again E^+, because the operator $\not{p} + mc$ does not have full rank, and thus does not map four linearly independent solutions onto another four linearly independent solutions).
- The negative energy solutions are thus

$$\psi^{(3)}(x) = e^{-\frac{i}{\hbar} p(E^-)\cdot x}\, u^{(3)}(p(E^-)) = \frac{e^{-\frac{i}{\hbar}(E^- t - \vec{p}\cdot\vec{x})}}{\sqrt{2mc^2(-E^- + mc^2)}} \begin{pmatrix} -cp^z \\ -c(p^x + ip^y) \\ -E^- + mc^2 \\ 0 \end{pmatrix}$$

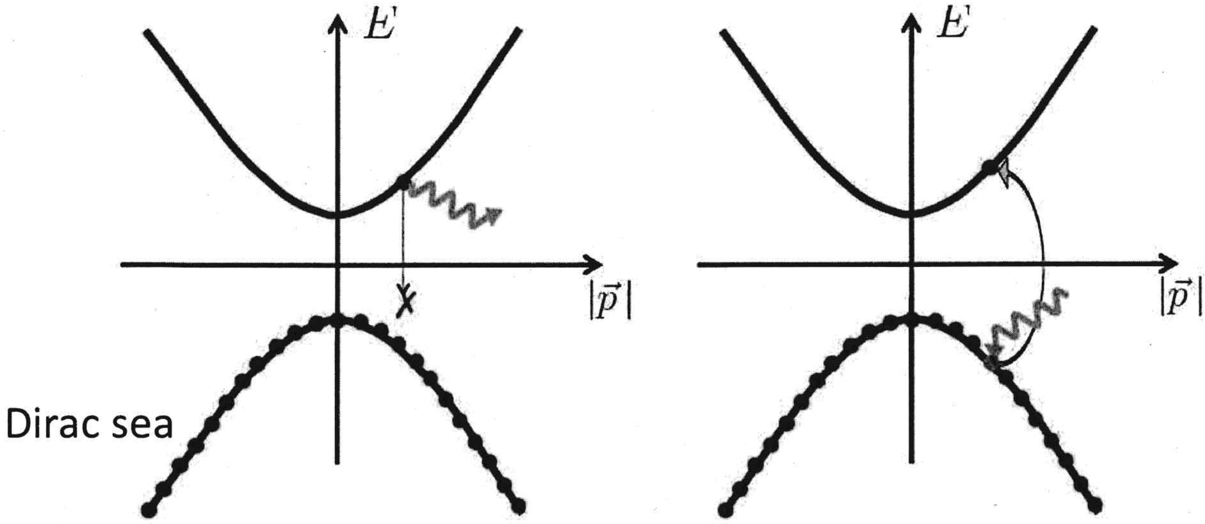
and

$$\psi^{(4)}(x) = \frac{e^{-\frac{i}{\hbar}(E^- t - \vec{p}\cdot\vec{x})}}{\sqrt{2mc^2(-E^- + mc^2)}} \begin{pmatrix} -c(p^x - ip^y) \\ cp^z \\ 0 \\ -E^- + mc^2 \end{pmatrix}.$$

- These solutions with negative energy are indeed necessary in order to span a complete basis for the spinor wave functions.
- However, like in the case of the Klein-Gordon equation this poses a problem; namely, it is unclear what the ground state of a free Dirac particle (e.g. an electron) is.

- To overcome this problem Dirac proposed in 1930 his <u>hole-theory</u>.
- This states that all states with negative energy are completely filled, which is (at least in principle) possible because Dirac particles are fermions (Dirac sea).
- This means that no particle with positive energy can decay under the emission of a photon into a negative energy state, because of the Pauli principle.
- Conversely, it should be possible to excite a particle with negative energy, e.g. by irradiating a photon with energy $+2\sqrt{\vec{p}^2c^2+m^2c^4}$, into one of the positive energy state.
- This creates a hole in the Dirac sea.
- Such absence of a particle in the Dirac sea is interpreted as an oppositely charged particle with positive energy.
- The excitation of a particle from the Dirac sea thus creates two particles with opposite charge and positive energy, which are interpreted as particle-anti-particle pair.

Hole-theory and Dirac sea



Skript zur Vorlesung
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(Quantenmechanik II)
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- Note, that for the Klein-Gordon equation, which describes bosons, such „Dirac sea" construction is not possible.
- Let us now construct the solutions for the anti-particles.
- To this end we construct the four-current density of the solutions for the Dirac equation.
- $\psi^{(1)}$ and $\psi^{(2)}$ lead to

$$(j^\mu) = \frac{1}{mc}\begin{pmatrix} \frac{E^+}{c} \\ \vec{p} \end{pmatrix}.$$

- $\psi^{(3)}$ and $\psi^{(4)}$ result in

$$(j^\mu) = \frac{1}{mc}\begin{pmatrix} -\frac{E^-}{c} \\ -\vec{p} \end{pmatrix},$$

and for these solutions the current density $\vec{j}$ points into the direction that is opposite to the momentum.
- The same is true for the phase velocity of the negative energy solutions, since $e^{-\frac{i}{\hbar}(\underset{\uparrow}{E^-}t - \vec{p}\cdot\vec{x})}$.
negative
- Inverting the direction of momentum in both solutions, therefore would lead to wave functions propagating along the direction of $\vec{p}$.

- Using from now on $E \equiv + \sqrt{\vec{p}^2 c^2 + m^2 c^4}$, this yields the following set of solutions for the Dirac equation:

<u>particle solutions</u>:

$$\psi_P^{(1)}(x) = e^{-\frac{i}{\hbar} p\cdot x} u^{(1)}(p) \quad , \quad \psi_P^{(2)}(x) = e^{-\frac{i}{\hbar} p\cdot x} u^{(2)}(p)$$

with

$$u^{(1)}(p) = \sqrt{\frac{E+mc^2}{2mc^2}} \begin{pmatrix} 1 \\ 0 \\ \frac{cp^z}{E+mc^2} \\ \frac{c(p^x+ip^y)}{E+mc^2} \end{pmatrix} , \quad u^{(2)}(p) = \sqrt{\frac{E+mc^2}{2mc^2}} \begin{pmatrix} 0 \\ 1 \\ \frac{c(p^x+ip^y)}{E+mc^2} \\ -\frac{cp^z}{E+mc^2} \end{pmatrix}$$

These solutions obey the equation

$$(\not{p} - mc)\, u(p) = 0 .$$

<u>anti-particle solutions</u>

$$\psi_A^{(1)}(x) = e^{\frac{i}{\hbar} p\cdot x} v^{(1)}(p) \quad , \quad \psi_A^{(2)}(x) = e^{\frac{i}{\hbar} p\cdot x} v^{(2)}(p)$$

with

$$v^{(1)}(p) = \sqrt{\frac{E+mc^2}{2mc^2}} \begin{pmatrix} \frac{c(p^x-ip^y)}{E+mc^2} \\ -\frac{cp^z}{E+mc^2} \\ 0 \\ 1 \end{pmatrix} , \quad v^{(2)}(p) = \sqrt{\frac{E+mc^2}{2mc^2}} \begin{pmatrix} \frac{cp^z}{E+mc^2} \\ \frac{c(p^x+ip^y)}{E+mc^2} \\ 1 \\ 0 \end{pmatrix}$$

These solutions obey the equation

$$(\not{p} + mc)\, v(p) = 0 .$$

- To conclude, we provide some useful relations for the spinors.

i) inner products:

$$[u^{(r)}(p)]^{+} u^{(s)}(p) = [v^{(r)}(p)]^{+} v^{(s)}(p) = \frac{E}{mc^2}\delta^{rs},$$

$$\bar{u}^{(r)}(p)\, u^{(s)}(p) = -\bar{v}^{(r)}(p)\, v^{(s)}(p) = \delta^{rs},$$

$$\bar{u}^{(r)} v^{(s)} = \bar{v}^{(r)} u^{(s)} = 0 .$$

ii) outer products (completeness relations):

$$\sum_{s=1}^{2} u^{(s)}(p)\, \bar{u}^{(s)}(p) = \frac{\not{p} + mc}{2mc},$$

$$\sum_{s=1}^{2} v^{(s)}(p)\, \bar{v}^{(s)}(p) = \frac{\not{p} - mc}{2mc} .$$

V. 6 Covariance of the Dirac equation

- In order to get an understanding of what covariance actually means, we begin with the Klein-Gordon equation, which can be written as

$$\left(\partial_\mu \partial^\mu + \left(\frac{mc}{\hbar}\right)^2\right) \psi(x) = 0 .$$

- The coordinates x and the derivatives refer to a specific intertial frame of reference, IS.

- An observer in a different inertial frame of reference, IS', would write the Klein-Gordon equation in exactly the same way:

$$\left(\partial'_\mu \partial'^\mu + \left(\frac{mc}{\hbar}\right)^2\right)\psi'(x') = 0 .$$

- The question is now how the wave functions $\psi(x)$ and $\psi'(x')$ are related to one another.

- Since it is possible to transform between different inertial frames of reference via the Lorentz-transform, it should also be possible to find a transformation law that directly connects the wave functions $\psi(x)$ and $\psi'(x')$, such that $\psi'(x')$ solves the Klein-Gordon equation in IS' when $\psi(x)$ solves the Klein-Gordon equation in IS.
- This property is referred to as <u>relativistic covariance</u>.

- The Klein-Gordon equation depends on $\partial_\mu \partial^\mu$ which is a Lorentz-scalar, and hence when transforming from IS to IS' one finds

$$\partial'_\mu \partial'^\mu = \partial_\mu \partial^\mu .$$

- The term $\left(\frac{mc}{\hbar}\right)^2$ is also a scalar and therefore the Klein-Gordon equation is indeed relativistically covariant.
- For the wave functions we find

$$\psi'(x') = \psi(x),$$

which is also reflected by the free solutions:

$$\psi(x) = e^{\frac{i}{\hbar}(\vec{p}\cdot\vec{x} - Et)} = e^{-\frac{i}{\hbar}p\cdot x} = e^{-\frac{i}{\hbar}p'x'} \equiv \psi'(x').$$

- For calculating the wave function in IS' it is just sufficient to transform the argument of the wave function via a Lorentz-transform, $x' = \Lambda x$.
- The wave function is thus a Lorentz-scalar, i.e. it has at the same space-time point the same value, no matter whether we are in IS or IS'.
- Let us now focus on the Dirac equation where the situation is a bit more involved.
- In the inertial frame of reference IS' is should read

$$(i\hbar\gamma^{\mu}\partial'_{\mu} - mc)\,\psi'(x') = 0.$$

- The problem is that $\gamma^\mu \partial_\mu$ is not a Lorentz-scalar, which is due to the fact that (γ^μ) is a vector of constant matrices and thus does not transform like a four-vector.
- This issue is fixed by the fact that the spinor ψ transforms in a non-trivial fashion, unlike the wave function of the Klein-Gordon equation.
- We make the ansatz

$$\psi'(x') = S(\Lambda)\psi(x).$$

- To determine the 4×4 transformation matrix $S(\Lambda)$ we multiply the Dirac equation from the left with $S(\Lambda)$ and write $\psi(x) = S^{-1}(\Lambda)\psi'(x')$.

$$(i\hbar\gamma^\mu\partial_\mu - mc)\psi(x) = 0$$

$$\hookrightarrow S(i\hbar\gamma^\mu\partial_\mu - mc)S^{-1}\psi'(x') = 0$$

$$\hookrightarrow (i\hbar\, S\gamma^\mu S^{-1}\partial_\mu - mc)\psi'(x') = 0$$

- If we find an S that satisfies

$$S\gamma^\mu S^{-1}\partial_\mu = \gamma^\nu \partial'_\nu$$

we have shown the covariance of the Dirac equation.

- Using $\partial'_\nu = \Lambda_\nu^{\ \mu} \partial_\mu$ we find that $S(\Lambda)$ is determined by the equation

$$S(\Lambda)\,\gamma^\mu\, S^{-1}(\Lambda) = \gamma^\mu \Lambda_\nu^{\ \mu}.$$

- Different Lorentz-transformations Λ thus give rise to a different transformation matrix S:

i) Lorentz-boost in x^1-direction

$$(\Lambda^\mu{}_\nu) = \begin{pmatrix} \gamma & -\beta\gamma & 0 & 0 \\ -\beta\gamma & \gamma & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \underset{=}{\beta = \tanh(\eta)} \begin{pmatrix} \cosh\eta & -\sinh\eta & 0 & 0 \\ \sinh\eta & \cosh\eta & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

$$\hookrightarrow S(\Lambda) = \begin{pmatrix} \cosh\frac{\eta}{2} & 0 & 0 & -\sinh\frac{\eta}{2} \\ 0 & \cosh\frac{\eta}{2} & -\sinh\frac{\eta}{2} & 0 \\ 0 & -\sinh\frac{\eta}{2} & \cosh\frac{\eta}{2} & 0 \\ -\sinh\frac{\eta}{2} & 0 & 0 & \cosh\frac{\eta}{2} \end{pmatrix}$$

ii) Boost in arbitrary direction, i.e. IS' moves with velocity $\vec{v}$ with respect to IS

$$S(\Lambda) = \exp\left(-\frac{\eta}{2}\frac{\vec{\alpha}\cdot\vec{v}}{|\vec{v}|}\right) = \mathbb{1}\cos\frac{\eta}{2} - \frac{\vec{\alpha}\cdot\vec{v}}{|\vec{v}|}\sinh\frac{\eta}{2}.$$

iii) Rotation about the x^3-axis by angle θ

$$(\Lambda^\mu{}_\nu) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos\theta & \sin\theta & 0 \\ 0 & -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

$\hookrightarrow \quad S(\Lambda) = \mathbb{1} \cos\frac{\Theta}{2} + i \Sigma^3 \sin\frac{\Theta}{2}$

Pauli matrix

with $\Sigma^3 = \begin{pmatrix} \sigma^3 & 0 \\ 0 & \sigma^3 \end{pmatrix}$

iv) Rotation about a general axis $\vec{n}$

$$S(\Lambda) = \exp\left(i \frac{\Theta}{2} \vec{\Sigma}\cdot\vec{n}\right) = \mathbb{1} \cos\frac{\Theta}{2} + i\vec{n}\cdot\vec{\Sigma} \sin\frac{\Theta}{2}$$

with $\vec{\Sigma} = \begin{pmatrix} \vec{\sigma} & 0 \\ 0 & \vec{\sigma} \end{pmatrix}$

Pauli matrices, $\vec{\sigma} = \begin{pmatrix} \sigma^1 \\ \sigma^2 \\ \sigma^3 \end{pmatrix}$

closely related to spin operator

- From the last expression one reads off that the spinor apparently returns to its original state only if one rotates by an angle 4π.
- Such behaviour is typical for spin-$\frac{1}{2}$-particles.
- Despite the fact that a spinor has a special behaviour under Lorentz-transformation, one can construct quantities with typical transformation behaviour when combining the spinor ψ with its Dirac-adjoint spinor $\bar{\psi}$.
- <u>Examples</u>:

  $\bar{\psi}(x)\psi(x)$ is a Lorentz-scalar

  $\bar{\psi}(x)\gamma^\mu\psi(x)$ is a four-vector

V.7 Spin

- In the Schrödinger equation spin needed to be introduced by hand, while the concept of spin emerges rather naturally in the Dirac equation.
- We define the spin operator

$$\vec{S} = \frac{\hbar}{2} \vec{\Sigma} = \frac{\hbar}{2} \begin{pmatrix} \vec{\sigma} & 0 \\ 0 & \vec{\sigma} \end{pmatrix},$$

whose components obey the angular momentum algebra

$$[S^i, S^j] = i\hbar S^k \varepsilon_{ijk} .$$

- Furthermore, $\vec{S}^2 = \frac{3}{4} \hbar^2 \mathbb{1}$.
- One can show that the Dirac Hamiltonian

$$H_{Dirac} = c \vec{\alpha} \cdot \vec{p} + \beta mc^2$$

does not commute with $\vec{S}$, i.e. $[H_{Dirac}, \vec{S}] = 0$.
- It also does not commute with the orbital angular momentum operator $\vec{L} = \vec{r} \times \vec{p}$.
- However, one can show that

$$[H_{Dirac}, \vec{L} + \vec{S}] = 0,$$

and thus the total angular momentum, $\vec{L} + \vec{S}$, is conserved for a particle that evolves under the free Dirac Hamiltonian.

- One can construct another, spin-related operator, with which H_{Dirac} commutes and according to whose eigenvalues states can be classified.
- This is the so-called <u>helicity-operator</u>

$$h(\vec{p}) = \frac{1}{2}\frac{\vec{\Sigma}\cdot\vec{p}}{|\vec{p}|} .$$

(note, that $\vec{p}$ is not an operator here)

- This operator corresponds to the projection of the spin onto the direction of the momentum.
- The eigenvalues of $h(\vec{p})$ are

$\lambda = \frac{1}{2}$: positive / right-handed helicity (the spin points into the direction of the momentum)

$\lambda = -\frac{1}{2}$: negative / left-handed helicity (the spin points opposite to the direction of the momentum)

- For the simple case $\vec{p} = |\vec{p}|\vec{e}_z$ we can write

$$h(\vec{p}) = \frac{1}{2}\Sigma^3 = \frac{1}{2}\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} .$$

- The spinors in the solution of the free Dirac equation with defined helicity are

$$u^{(1)}(p) = \sqrt{\frac{E+mc^2}{2mc^2}}\begin{pmatrix} 1 \\ 0 \\ \frac{c|\vec{p}|}{E+mc^2} \\ 0 \end{pmatrix} , \quad u^{(2)}(p) = \sqrt{\frac{E+mc^2}{2mc^2}}\begin{pmatrix} 0 \\ 1 \\ 0 \\ -\frac{c|\vec{p}|}{E+mc^2} \end{pmatrix}$$

$$v^{(1)}(p) = \sqrt{\frac{E+mc^2}{2mc^2}} \begin{pmatrix} 0 \\ -\frac{c|\vec{p}|}{E+mc^2} \\ 0 \\ 1 \end{pmatrix}, \quad v^{(2)}(p) = \sqrt{\frac{E+mc^2}{2mc^2}} \begin{pmatrix} \frac{c|\vec{p}|}{E+mc^2} \\ 0 \\ 1 \\ 0 \end{pmatrix}.$$

- They are simultaneous eigenstates of H_{Dirac} and $h(p)$:

$$\left.\begin{aligned} \frac{1}{2}\frac{\vec{\Sigma}\cdot\vec{p}}{|\vec{p}|}u^{(1)}(p) &= +\frac{1}{2}u^{(1)}(p) \\ \frac{1}{2}\frac{\vec{\Sigma}\cdot\vec{p}}{|\vec{p}|}u^{(2)}(p) &= -\frac{1}{2}u^{(2)}(p) \end{aligned}\right\} \text{particle states}$$

$$\left.\begin{aligned} \left(-\frac{1}{2}\frac{\vec{\Sigma}\cdot\vec{p}}{|\vec{p}|}\right)v^{(1)}(p) &= +\frac{1}{2}v^{(1)}(p) \\ \left(-\frac{1}{2}\frac{\vec{\Sigma}\cdot\vec{p}}{|\vec{p}|}\right)v^{(2)}(p) &= -\frac{1}{2}v^{(2)}(p) \end{aligned}\right\}$$

antiparticle states, where we use $\vec{\Sigma} \to -\vec{\Sigma}$, since $\vec{S} \to -\vec{S}$ (we already changed $\vec{p} \to -\vec{p}$ before)

- For antiparticles we have $\vec{p} \to -\vec{p}$ and $\vec{S} \to -\vec{S}$.

V.8 The Dirac equation with an electromagnetic field

- We want to investigate the Dirac equation in the presence of a vector potential $\vec{A}(\vec{x},t)$ and a scalar potential $\phi(\vec{x},t)$.
- A (classical) particle couples to these potentials via its charge, q, which is reflected by the minimal substitution

$$E \to E - q\phi \quad , \quad \vec{p} \to \vec{p} - q\vec{A}.$$

- Using the correspondence principle this amounts to
$$i\hbar\frac{\partial}{\partial t} \to i\hbar\frac{\partial}{\partial t} - q\phi \ , \quad \frac{\hbar}{i}\nabla \to \frac{\hbar}{i}\vec{\nabla} - q\vec{A} \ ,$$
which, by making use of the four-vectors $(p^\mu) = (\frac{E}{c}, \vec{p})$ and $(A^\mu) = (\phi/c, \vec{A})$, can be compactly written as
$$\hat{p}^\mu \to \hat{p}^\mu - qA^\mu \ .$$
- Making this substitution, the Dirac equation becomes
$$(i\hbar\not{\partial} - q\not{A}(x) - mc)\psi(x) = 0 \ .$$
- Before continuing, let us briefly come back to the construction of anti-particle states:
- One can show, that the so-called <u>charge conjugated spinor</u>
$$\psi_c(x) = i\gamma^2\psi^*(x) = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \\ 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}\psi(x)$$
satisfies the above equation, but with charge $-q$.
- Moreover, one finds that the charge conjugation operation actually yields the anti-particle spinors when applied to the particle spinors.
- From this follows that particles and anti-particles carry opposite charges

- Let us now focus on the non-relativistic limit of the Dirac equation.
- We start with the non-covariant form

$$i\hbar \frac{\partial}{\partial t}\psi(\vec{x},t) = \Big[c\vec{\alpha}\cdot\underbrace{\Big(\frac{\hbar}{i}\nabla - q\vec{A}\Big)}_{\vec{\pi}\,=\,\vec{p}-q\vec{A}\ \ldots\ \text{kinetic momentum}} + q\phi + \beta mc^2 \Big]\psi(\vec{x},t)$$

- We now make the following ansatz for the spinor:

$$\psi = \begin{pmatrix}\tilde{\varphi}\\ \tilde{\chi}\end{pmatrix} = \underbrace{e^{-\frac{i}{\hbar}mc^2 t}}_{\text{we separate this fast oscillation}}\begin{pmatrix}\varphi\\ \chi\end{pmatrix}$$

- The two-component spinors are „slowly" evolving, i.e. on timescales that are much longer than $\frac{\hbar}{mc^2}$.
- Inserting the ansatz into the Dirac equation yields

$$mc^2\begin{pmatrix}\varphi\\ \chi\end{pmatrix} + i\hbar\frac{\partial}{\partial t}\begin{pmatrix}\varphi\\ \chi\end{pmatrix} = \left(c\vec{\alpha}\cdot\vec{\pi} + q\phi + \beta mc^2\right)\begin{pmatrix}\varphi\\ \chi\end{pmatrix},$$

which becomes after using the explicit forms of the α^i and β-matrices

$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix}\varphi\\ \chi\end{pmatrix} = c\,\vec{\sigma}\cdot\vec{\pi}\begin{pmatrix}\chi\\ \varphi\end{pmatrix} + q\phi\begin{pmatrix}\varphi\\ \chi\end{pmatrix} - 2mc^2\begin{pmatrix}0\\ \chi\end{pmatrix}.$$

- The second row is dominated by the last term: $|mc^2\chi| \gg |q\phi\chi|, |\hbar\frac{\partial}{\partial t}\chi|$.

- Neglecting the time derivative and the term proportional to $q\phi$, the second line becomes an algebraic equation, which is solved by

$$\chi = \frac{\vec{\sigma}\cdot\vec{\pi}}{2mc}\varphi$$

φ: upper / large spinor component

χ: lower / small spinor component

- This relation shows, that in the non-relativistic limit $|\chi| \ll |\varphi|$, since here the velocity $|\vec{v}| \approx \left|\frac{\vec{\pi}}{m}\right|$ should be much smaller than the speed of light.

- We can now eliminate χ from the upper line, which yields the equation of motion for the upper spinor component

$$i\hbar \frac{\partial}{\partial t}\varphi(\vec{x},t) = \left[\frac{1}{2m}(\vec{\sigma}\cdot\vec{\pi})^2 + q\phi\right]\varphi(\vec{x},t)$$

- One can show that

$$(\vec{\sigma}\cdot\vec{\pi})(\vec{\sigma}\cdot\pi) = \vec{\pi}^2 + i\sigma\cdot(\vec{\pi}\times\vec{\pi}).$$

- For the x-component of the cross product of operators in the second term one finds

$$\begin{aligned}
(\vec{\pi}\times\vec{\pi})^x\varphi &= (\pi^y\pi^z - \pi^z\pi^y)\varphi \\
&= ((\hat{p}^y - qA^y)(\hat{p}^z - qA^z) - (\hat{p}^z - qA^z)(\hat{p}^y - qA^y))\varphi \\
&= q\frac{\hbar}{i}\left(-\frac{\partial}{\partial y}A^z - A^y\frac{\partial}{\partial z} + \frac{\partial}{\partial z}A^y + A^z\frac{\partial}{\partial y}\right)\varphi \\
&= q\frac{\hbar}{i}\varphi\left(-\frac{\partial A^z}{\partial y} + \frac{\partial A^y}{\partial z}\right)\varphi = i\hbar q B^x\varphi
\end{aligned}$$

- Following an analogous calculation for the other components leads to the equation

$$i\hbar \frac{\partial}{\partial t} \varphi(\vec{x},t) = \left[\frac{1}{2m}(\vec{p}-q\vec{A})^2 - \frac{q\hbar}{2m}\vec{\sigma}\cdot\vec{B} + q\phi\right]\varphi(\vec{x},t).$$

- For a homogeneous magnetic field, $q=-e$ and the Coulomb potential $q\phi = -\frac{e^2}{4\pi\varepsilon_0|\vec{r}|}$ this leads to the Pauli-equation for the Hydrogen atom (using $(\vec{p}+e\vec{A})^2 \approx \vec{p}^2 + e\vec{B}\cdot\vec{L}$)

$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix}\psi_\uparrow\\ \psi_\downarrow\end{pmatrix} = \left[\frac{\vec{p}^2}{2m} - \frac{e^2}{4\pi\varepsilon_0|\vec{r}|} + \frac{\mu_B}{\hbar}\vec{L}\cdot\vec{B} + \frac{g_s}{2}\mu_B\vec{\sigma}\cdot\vec{B}\right]\begin{pmatrix}\psi_\uparrow\\ \psi_\downarrow\end{pmatrix}$$

with the Bohr magneton $\mu_B = \frac{e\hbar}{2m}$ and the Landé factor $g_s = 2$.

- The prediction of g_s is a huge success of Dirac's theory.
- One can systematically improve the approximation describing the non-relativistic limit, e.g. through the so-called Foldy-Wouthuysen transformation.
- This leads for time-independent fields to

$$i\hbar\frac{\partial}{\partial t}\varphi(\vec{x},t) = \left[\frac{1}{2m}(\vec{p}-q\vec{A})^2 - \frac{q\hbar}{2m}\vec{\sigma}\cdot\vec{B} + q\phi - \frac{\vec{p}^4}{8m^3c^2} - \frac{q\hbar}{4m^2c^2}\vec{\sigma}\cdot(\vec{E}\times(\vec{p}-q\vec{A})) - \frac{q\hbar^2}{8m^2c^2}(\vec{\nabla}\cdot\vec{E})\right]\varphi(\vec{x},t).$$

- The three terms in the second row also contribute when there is only a scalar potential present and $\vec{A}=0$.

i) The term $\frac{\vec{p}^4}{8m^3c^2}$ is the first <u>relativistic correction</u> stemming from the expansion of the relativistic energy-momentum relation $E=\sqrt{\vec{p}^2c^2+m^2c^4}$

ii) The second term in the second line becomes with $q=-e$ and the Coulomb potential $(-e)\phi = -\frac{e^2}{4\pi\varepsilon_0|\vec{r}|}$

$$\frac{e\hbar}{4m^2c^2}\vec{\sigma}\cdot(\vec{E}\times\vec{p}) = -\frac{e\hbar}{4m^2c^2}\frac{d\phi}{dr}\frac{1}{r}\vec{\sigma}\cdot(\vec{r}\times\vec{p})$$
$$= \frac{\hbar}{4m^2c^2}\frac{e^2}{4\pi\varepsilon_0 r^3}\vec{\sigma}\cdot\vec{L}$$
$$= \frac{e^2}{4\pi\varepsilon_0 m^2c^2}\frac{\vec{L}\cdot\vec{S}}{2r^3}.$$

This is the <u>spin-orbit coupling</u> term with the correct „Thomas"-factor $\frac{1}{2}$!

iii) For the last term we use Maxwell's equation
$$\nabla\cdot\vec{E} = \frac{\rho}{\varepsilon_0} = \frac{e}{\varepsilon_0}\delta^{(3)}(\vec{r}),$$
with $\rho = e\,\delta^{(3)}(\vec{r})$ being the charge density of the point-like nucleus.

With this the term becomes

$$\frac{e^2\hbar^2}{8m^2c^2\varepsilon_0}\,\delta^{(3)}(r)\,,$$

which is the so-called <u>Darwin term</u>.

- Finally, we remark that the Dirac equation can actually be solved exactly in the presence of the Coulomb potential.
- This yields the energy eigenvalues

$$\underset{\substack{\text{principal}\\\text{quantum}\\\text{number}}}{E_{n}}\underset{\substack{\text{total}\\\text{angular}\\\text{momentum}\\\text{quantum}\\\text{number}}}{{}_{j}} = \frac{mc^2}{\sqrt{1+\dfrac{\alpha_{FS}^2}{\left(n-(j+\frac{1}{2})+\sqrt{(j+\frac{1}{2})^2-\alpha_{FS}^2}\right)^2}}}\,.$$

- Expanding in the fine-structure constant $\alpha_{FS} = \frac{e^2}{4\pi\varepsilon_0\hbar c} \approx \frac{1}{137}$ yields

$$E_{n,j} = mc^2\left[1-\frac{\alpha_{FS}^2}{2n^2}+\frac{\alpha_{FS}^4}{2n^4}\left(\frac{3}{4}-\frac{n}{j+\frac{1}{2}}\right)+\mathcal{O}(\alpha_{FS}^6)\right]$$

$$= mc^2 \underbrace{-\frac{E_{Ry}}{n^2}}_{\substack{\text{Rydberg}\\\text{energies}}} + \underbrace{\frac{\alpha_{FS}^2 E_{Ry}}{n^4}\left(\frac{3}{4}-\frac{n}{j+\frac{1}{2}}\right)}_{\text{hydrogen fine-structure}} + \mathcal{O}(\alpha_{FS}^6)$$

$$E_{Ry} = \frac{1}{2}\alpha_{FS}^2 mc^2 \approx 13.6\ \mathrm{eV}.$$