Dirac equation

Victor Kärcher

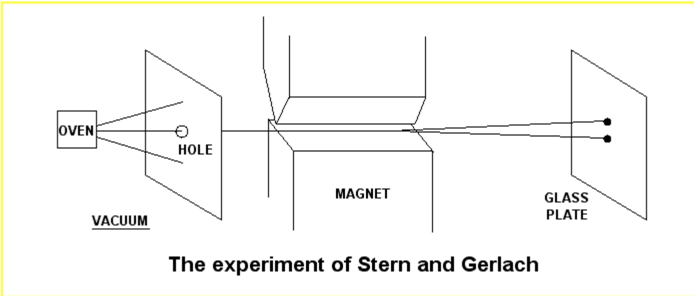
07th of January 2015

Contents

1 Introduction

In 1922 the german physicists Otto Stern and Walter Gerlach showed in their experiment that the electron has a spin. This experiment involves sending a beam of particles through an inhomogeneous magnetic field and observing their deflection.

Figure 1: Stern-Gerlach experiment[3]



The particles they used in 1922 were silver atoms. At this time phyisicists knew that the quantum number l of the 5s electron is equal to zero and that the atom is electrical neutral. So the expectation was to only see one path. But as shown in Figure 1 this beam has been divided into two parts. The explanation was that the electron possesses an intrinsic angular momentum called "spin", which is similar to the angular momentum of a classically spinning object. It only takes certain quantized values, which is $\frac{\hbar}{2}$ for an electron.
Based on these considerations there has to be an equation describing the spin mathematically and it is called the "Dirac equation".

2 Relativistic theory of the electron

The Dirac equation is a linearization of the relativistic engergy momentum theorem:

$$E^2 = c^2\vec{p}^2 + m_e^2 c^4,$$

where $\vec{p}$ is the relativistic momentum and m_e the mass of a free electron:

$$\vec{p} = \gamma m_e \vec{v} \qquad \gamma = \left(1 - \frac{v^2}{c^2}\right)^{-\frac{1}{2}},$$

where $\vec{v}$ is the velocity of an electron and c the speed of light.
With the aid of the correspondic principle, the following connections are known:

$$\vec{p} \to \frac{\hbar}{i}\nabla; \quad E \to i\hbar\frac{\partial}{\partial t}.$$

This quantization should be equal in all reference systems. In other words it should be invariant under Lorentz-Transformation. Therefore the classical relativistic energy momentum theorem can be written as:

$$p^\mu p_\mu = m_e c^2. \tag{1}$$

p^μ is the contravariant momentum operator in four dimensions:

$$p^\mu = \left(\gamma m_e \vec{v}, i\frac{E}{c}\right).$$

Accordingly the contravariant gradient is given by:

$$\partial^\mu = \left(-\nabla, \frac{i}{c}\frac{\partial}{\partial t}\right),$$

so under the condition of the correspondic principle, the momentum operator is promoted to this four dimensional gradient:

$$p^\mu \to i\hbar\partial^\mu. \tag{2}$$

Along with the relativistic correspondic principle the squared norm of the momentum operator (1) we receive:

$$p^\mu p_\mu \to -\hbar^2 \partial^\mu \partial_\mu = \hbar^2 \Box. \tag{3}$$

$\Box$ is called the *d'Alembert-opereator*,

$$\Box = \Delta - \frac{1}{c^2}\frac{\partial^2}{\partial t^2} \qquad (\Delta : \mathrm{Laplace - Operator}).$$

In quantum mechanics we want to know how an operator changes the state of a physical particle, which is in this case the electron. Thus it appears that the state is given by a four dimensional wavefuction $|\psi(\vec{r}, t)\rangle$ and this wavefunction depends on the contravariant space vector $x^\mu \equiv (x, y, z, ict)$. Mathematically we get:

$$\left(\Delta - \frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \frac{m_e c^2}{\hbar^2}\right)|\psi(\vec{r}, t\rangle = 0. \tag{4}$$

In this form the equation is called *Klein-Gordon-Equation.* But there are some problems with this equation:

1. It only describes particles without spin.

2. It is a differential equation in second order.

3. It may have a negative probability density in some cases.

4. The solution also involves negative energies.

However, Dirac's idea was to linearize the relativisitic energy momentum theorem (1) in the following way:

$$\left(E - c\sum_i \hat{\alpha}_i p_i - \hat{\beta} m_e c^2\right)\left(E + c\sum_j \hat{\alpha}_j p_j + \hat{\beta} m_e c^2\right) = 0, \quad i,j \in (x,y,z). \tag{5}$$

By expanding equation (5), we realize that the new elements $\hat{\alpha}$,$\hat{\beta}$ have to fullfil the following relations:

$$[\hat{\alpha}_i, \hat{\alpha}_j]_+ = 2\delta_{ij} id_n, \tag{6}$$

$$[\hat{\alpha}_i, \hat{\beta}]_+ = 0 \qquad \hat{\beta}^2 = id_n. \tag{7}$$

The Pauli spin matrices are given by:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

The anticommutator for two different components of the Pauli matrices look simmilar to (6):

$$[\sigma_i, \sigma_j]_+ = 2\delta_{ij} id_2. \tag{8}$$

$\hat{\alpha}$ and $\hat{\beta}$ should be at least $4x4$-matrices. They might look like:

$$\alpha = \begin{pmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & 0 \end{pmatrix} \qquad \hat{\beta} = \begin{pmatrix} id_2 & 0 \\ 0 & -id_2 \end{pmatrix}.$$

3 Dirac equation

3.1 Dirac equation for the free electron

Every solution of the equation:

$$\left(E \mp c\sum_i \hat{\alpha}_i p_i \mp \hat{\beta} m_e c^2\right) = 0 \tag{9}$$

is a solution for (5). With the aid of the correspondic principle the linearization can be written as

$$\left(i\hbar\frac{\partial}{\partial t} + i\hbar c\hat{\alpha}\cdot\nabla - \hat{\beta} m_e c^2\right)|\psi(\vec{r},t)\rangle = 0 \tag{10}$$

and it is called the **Dirac equation for the free electron**. In its free form it describes all spin-$\frac{1}{2}$ massive particles for which parity is a symmetry such as elctrons and quarks.[4]

In order to get the old structure of the nonrelativistic Schrödinger equation we introduce the **Dirac-operator**:

$$H_D^{(0)} = c\hat{\alpha} \cdot \vec{p} + \hat{\beta} m_e c^2. \tag{11}$$

Then the Dirac equation can be written in a time dependent and a time independent form:

1. time dependent: $i\hbar\frac{\partial}{\partial t} |\psi(\vec{r},t)\rangle = H_D^{(0)} |\psi(\vec{r},t)\rangle$
2. time independet: $E |\psi(\vec{r},t)\rangle = H_D^{(0)} |\psi(\vec{r},t)\rangle$.

The relativistic theory involves the equality of space and time coordinates. So the Schrödinger equation should be symmetric in space and time coordinates, in other words it has to be a differential equation in first order, which is realized by the Dirac equation.

3.2 Dirac equation for an electron in a magnetic field

As we saw in the experiment of Stern-Gerlach, there is a connection between this intrinsic angular momentum and a magnectic field. Therefore we take the usual substitution:

$$\vec{p} \to \vec{p} + e\vec{A}; \qquad E \to E + e\phi,$$

where $\vec{A}$ is a vector potential and ϕ is a scalar potential. In contravariant form the potential looks like:

$$p^\mu \to p^\mu + eA^\mu; \qquad A^\mu = \left(\vec{A}, \frac{i}{c}\phi\right). \tag{12}$$

Then the **Dirac equation for an electron in a magnetic field** is given by:

$$\left[i\hbar\frac{\partial}{\partial t} - c\hat{\alpha} \cdot \left(\frac{\hbar}{i} + e\vec{A}(\vec{r},t)\right) - \hat{\beta} m_e c^2 + e\phi(\vec{r},t)\right] |\psi(\vec{r},t)\rangle = 0 \tag{13}$$

and the **Dirac-operator for an electron in a magnetic field** looks like:

$$H_D^{em} = c\hat{\alpha} \cdot (\vec{p} + e\vec{A}) + \hat{\beta} m_e c^2 - e\phi. \tag{14}$$

3.3 Dirac equation in its covariant form

For this equation we do not use the bra-ket-form anymore. We switch to ψ and ψ^*. The first step to get the covariant formula is to multiply the Dirac Equation

$$i\hbar\partial_t\psi = \frac{\hbar}{i} c\hat{\alpha}\nabla\psi + \hat{\beta} m_e c^2\psi \tag{15}$$

with $\frac{1}{c}\hat{\beta}$ and due to $\hat{\beta}^2 = id_4$ we get

$$i\hbar[\hat{\beta}\partial_0 + \hat{\beta}\hat{\alpha}\nabla]\psi - m_e c\psi = 0. \tag{16}$$

We can write this equation in a short form, if we use the new matrices γ^μ:

$$\gamma^0 := \hat{\beta} \qquad \gamma^k := \hat{\beta}\alpha_k, \quad (k = 1, 2, 3). \tag{17}$$

So the **Dirac equation in its covariant form** is

$$(\hbar\gamma^\mu \partial_\mu - m_e c)\psi = 0. \tag{18}$$

However, this equation is not really covariant because the γ^μ are not components of a vector in four dimensions but they are constant matrices. In the absence of these 'real' covariance the transformation into another reference system is not given by:

$$\gamma'^\mu = \Lambda^\mu_\nu \gamma^\nu.$$

3.4 Probability density

The definition of the conjugated transposed wavefunction is

$$\psi^\dagger := (\psi_1^*, \psi_2^*, \psi_3^*, \psi_4^*) = (\psi^*)^T. \tag{19}$$

Then we multiply the Dirac equation (10) with $\psi^\dagger$ and get

$$i\hbar\psi^\dagger\dot{\psi} = \frac{\hbar}{i}c\psi^\dagger\hat{\alpha} \cdot \nabla\psi + m_e c^2 \psi^\dagger \beta\psi. \tag{20}$$

The next step is to do the same thing with the Dirac equation in conjugated form

$$-i\hbar\dot{\psi}^\dagger = -\frac{\hbar}{i}c(\nabla\psi^\dagger)\hat{\alpha}\psi + m_e c^2 \hat{\beta}\psi \tag{21}$$

and multiply (21) with ψ:

$$-i\hbar\dot{\psi}^\dagger\psi = -\frac{\hbar}{i}c(\nabla\psi^\dagger)\alpha\psi + m_e c^2 \psi^\dagger\hat{\beta}\psi. \tag{22}$$

Now we calculate the difference between (20) and (22):

$$\frac{\partial}{\partial t}(\psi^\dagger\psi) = -c\nabla(\psi^\dagger\hat{\alpha}\psi) \tag{23}$$

and we get the continuity equation:

$$\frac{\partial}{\partial t}\rho + \nabla\vec{j} = 0, \tag{24}$$

where the probability density is always postive,

$$\rho = \psi^\dagger\psi = \sum_i^4 \psi_i^*\psi_i \tag{25}$$

and $\vec{j} = c\psi^\dagger\hat{\alpha}\psi$ is the current density. The thing with the negative probability density is solved. However the dilemma with the occuring negative energies hasn't been solved yet. Therefore we have to look at the eigenvalue problem.

4 Solutions for the free Dirac equation

The eigenvalue problem is given by

$$det(H_D^{(0)} - E \cdot id_4) = 0, \tag{26}$$

where the solutions are

$$E_\pm = \pm\sqrt{c^2\vec{p}^2 + m_e^2 c^4}. \tag{27}$$

The positive energy is the classical relativistic energy momentum theorem. But there is also a negative solution. In the Klein-Gordon equation the negative energy was a solution for an antiparticle without spin. But are there antiparticles for particles with spin?
The ansatz for the Dirac equation is a four dimensional plane wave:

$$|\psi(\vec{r},t)\rangle = \vec{a} \cdot e^{\frac{i}{\hbar}p^\mu x_\mu} = \vec{a} e^{\frac{i}{\hbar}(\vec{p}\vec{r} - Et)}, \tag{28}$$

where $|\psi(\vec{r},t)\rangle$ or $\vec{a}$ is a **Dirac-Spinor**. For both eigenvalues there are two eigenspinors $\vec{a}_{1,2}$:

$$\hat{a}_1^{(+)} = d \begin{pmatrix} 1 \\ 0 \\ cp_z/\hat{E} \\ cp_+/\hat{E} \end{pmatrix} \qquad \hat{a}_2^{(+)} = d \begin{pmatrix} 0 \\ 1 \\ cp_-/\hat{E} \\ -cp_z/\hat{E} \end{pmatrix} \tag{29}$$

$$\hat{a}_1^{(-)} = d \begin{pmatrix} -cp_z/\hat{E} \\ -cp_+/\hat{E} \\ 1 \\ 0 \end{pmatrix} \qquad \hat{a}_2^{(-)} = d \begin{pmatrix} -cp_-/\hat{E} \\ cp_z/\hat{E} \\ 0 \\ 1 \end{pmatrix}, \tag{30}$$

where $\hat{E} = E_+ + m_e c^2$ and $p_\pm = p_1 \pm ip_2$. d is a constant which we get from the squared norm:

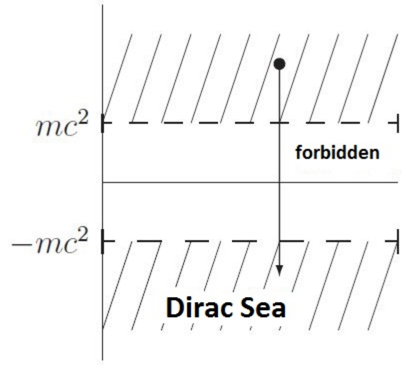
$$d = \frac{m_e c^2 + E_+}{\sqrt{(m_e c^2 + E_+)^2 + c^2\vec{p}^2}} = \frac{1}{\sqrt{1 + \frac{c^2\vec{p}^2}{\hat{E}^2}}} \quad \xrightarrow{v \ll c} \quad 1. \tag{31}$$

Every linear combination of (29) and (30) is a solution for the free Dirac equation.

4.1 Dirac sea

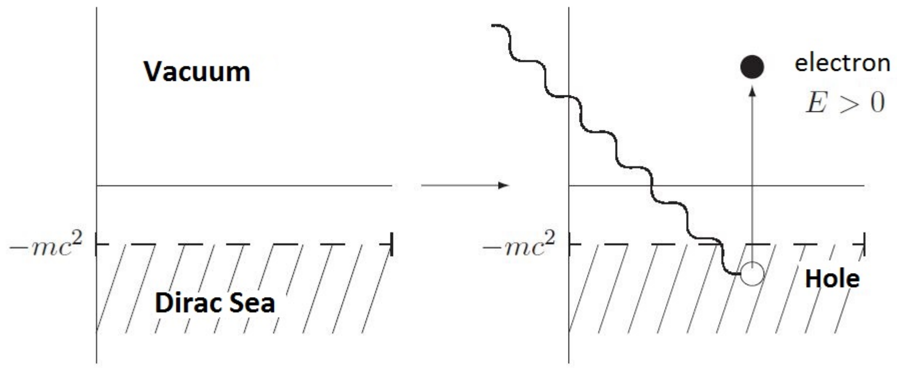
Dirac's idea to solve the dilemma with the negative energy eigenvalues was to introduce a concept where the states with E_- are fully staffed with electrons.

Figure 2: Dirac Sea[2]



So the transition for an electron with E_+ to the state with E_- is forbidden. For example a fully occupied state in an atom does not allow an extra particle in this state, too. At this time the Pauli principle already exists.
But a photon can transfer an electron with negative Energy E_- to a state with positive Energy E_+.

Figure 3: Transition from E_- to E_+[2]



Then there is left a hole with the same mass as an electron but with a positive charge. So this can not be a proton because $m_{proton} \gg m_e$. In 1930 Carl D. Anderson located this particle called positron in an experiment.

5 References

[1] W.Nolting *Grundkurs Theoretische Physik 5 Quantenmechanik Teil2: Methoden und Anwendungen*

[2] G. Münster *Skript zur Einführung in die Quantenfeldtheorie Wintersemester 2011/2012 Vorlesungsmitschrift von Burkhard Echtermeyer*

[3] `http://www.google.de/imgres?imgurl=http%3A%2F%2Fwww.physics.rutgers.edu%2F~zrwan%2Fphysics%2FStern-Gerlach%2FThe-Stern-Gerlach-experiment.gif&imgrefurl=http%3A%2F%2Fwww.physics.rutgers.edu%2F~zrwan%2Fphysics%2F&h=297&w=696&tbnid=AhavwREbZ1nalM%3A&zoom=1&docid=cz4EdkZjoQGRKM&ei=b6DLVKDbM8iwUaHcgugF&tbm=isch&iact=rc&uact=3&dur=113&page=1&start=0&ndsp=35&ved=0CEYQrQMwDA`
Date:30th of January 2015

[4] `http://en.wikipedia.org/wiki/Dirac_equation`
Date:3th of January 2015

[5] W.Nolting *Grundkurs Theoretische Physik 4 Spezielle Relativitätstheorie, Thermodynamik*