2° The Dirac equation

a) Derivation

Dirac (1928) postulates the following requirements for a consistent relativistic wave equation:

(i) First order in time: $i\hbar\, \partial_t \Psi = H \Psi$

This guarantees conservation of probability, because the time evolution operator $U = \exp(-\frac{i}{\hbar} t H)$ is unitary (Sect. I.1°), provided H is Hermitian.

(ii) Linear in momentum: Since momentum is represented by first order spatial derivatives, the relativistic symmetry between space and time, together with (i), requires that H is linear in p_k:

D
$$H = c\, \vec{\alpha} \cdot \vec{p} + \beta m c^2 =$$
$$= -i\hbar c\, \alpha^k \partial_k + \beta m c^2$$

with constant entities α^k, β.

(iii) Relativistic energy-momentum relation holds for H^2:

$$H^2 \overset{!}{=} c^2 |\vec{p}|^2 + m^2 c^4 = -\hbar^2 c^2 \nabla^2 + m^2 c^4 \mathbb{1}$$

Using the ansatz D this implies

$$H^2 = (-i\hbar c\, \alpha^k \partial_k + \beta m c^2)(-i\hbar c\, \alpha^l \partial_l + \beta m c^2) =$$

$$= -\hbar^2 c^2 \sum_{k,l=1}^{3} \alpha^k \alpha^l \partial_k \partial_l -$$

$$- i\hbar m c^3 \left(\alpha^k \beta + \beta \alpha^k \right) \partial_k + \beta^2 m^2 c^4 .$$

The first term contains diagonal and non-diagonal contributions:

$$\sum_{k,l=1}^{3} \alpha^k \alpha^l \partial_k \partial_l = \sum_{k=1}^{l} (\alpha^k)^2 \partial_k^2 + \frac{1}{2} \sum_{\substack{k,l=1 \\ k \neq l}}^{3} (\alpha^k \alpha^l + \alpha^l \alpha^k) \partial_k \partial_l$$

$$\Rightarrow H^2 = \underbrace{- \hbar^2 c^2 (\alpha^k)^2 \partial_k^2 + m^2 c^4 \beta^2}_{\stackrel{!}{=} -\hbar^2 c^2 \nabla^2 + m^2 c^4 \mathbb{1} = H_{KG}} -$$

$$\left. \begin{array}{l} - \frac{1}{2} \hbar^2 c^2 \sum\limits_{\substack{k,l=1 \\ k \neq l}}^{3} (\alpha^k \alpha^l + \alpha^l \alpha^k) \partial_k \partial_l - \\ \\ - i\hbar m c^3 \left(\alpha^k \beta + \beta \alpha^k \right) \partial_k \end{array} \right\} \stackrel{!}{=} 0$$

Thus the α^k, β have to satisfy

$$\left| \begin{array}{l} \{\alpha^k, \alpha^l\} = \alpha^k \alpha^l + \alpha^l \alpha^k = 2 \delta_{kl} \mathbb{1} \\ \{\alpha^k, \beta\} = 0 \qquad\qquad \beta^2 = \mathbb{1} \end{array} \right| \quad (*)$$

They cannot be numbers, but must be matrices acting on an <u>N-component spinor</u>:

$$i\hbar\, \partial_t \psi = H\psi\,, \qquad \psi = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_N \end{pmatrix}$$

What is the minimal value of N?

(i) $(\alpha^k)^2 = \beta^2 = \mathbb{1} \Rightarrow$ the eigenvalues of α^k, β are ± 1

(ii) $\alpha^k \beta = -\beta \alpha^k \Rightarrow \alpha^k = -\beta \alpha^k \beta$

$$\Rightarrow \mathrm{Tr}(\alpha^k) = -\mathrm{Tr}(\beta\alpha^k\beta) = -\mathrm{Tr}(\beta^2\alpha^k) =$$
$$= -\mathrm{Tr}(\alpha^k)$$

$$\Rightarrow \mathrm{Tr}(\alpha^k) = \mathrm{Tr}(\beta) = 0$$

It follows from (i) and (ii) that N must be even.

$N=2$: There are 3 mutually anticommuting, Hermitian matrices given by the Pauli matrices (exercise 2.1)

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

but we need 4!

$N=4$: The following 4×4 matrices satisfy $\circledast$:

$$\alpha^k = \begin{pmatrix} 0 & \sigma^k \\ \sigma^k & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} \mathbb{1}_2 & 0 \\ 0 & -\mathbb{1}_2 \end{pmatrix}$$

with $\mathbb{1}_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$.

b) Continuity equation

To define the probability density ρ and the corresponding current $\vec{j}$, we introduce the adjoint spinor

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

Then the the density and current defined by

$$\left.\begin{aligned} \rho &= \psi^\dagger \psi = \sum_{j=1}^{4} \psi_j^* \psi_j \\ j^k &= c\, \psi^\dagger \alpha^k \psi \end{aligned}\right\}$$

satisfy the continuity equation

$$\partial_t \rho + \nabla \cdot \vec{j} = 0$$ proof in exercise

With the four-current $j^\mu = (c\rho, j^k)$

this can be written as

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

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c) Covariant formulation

To make the space-time symmetry of the Dirac equation more conspicuous, we write it in the form

$$\Big(\underbrace{-i\hbar\,\partial_t}_{= i\hbar c\,\partial_0} - i\hbar c\,\alpha^k\,\partial_k + \beta m c^2\Big)\psi = 0$$

Multiply by β:

$$\left(- i\hbar c\beta\,\partial_0 - i\hbar c\,\alpha^k\,\partial_k + m c^2\right)\psi = 0$$

With the definition $\gamma^0 = \beta\ ,\ \gamma^k = \beta\alpha^k$ this yields

$$\left(-i\hbar c\,\gamma^\mu\,\partial_\mu + m c^2\right)\psi = 0$$

The γ^μ satisfy the anticommutation relations

$$\{\gamma^\mu, \gamma^\nu\} = 2 g^{\mu\nu}\,\mathbb{1}$$ exercise

3° Free particle solutions

We consider momentum eigenstates

$$\psi_{\vec p}(\vec r,t) = \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{pmatrix} e^{-\frac{i}{\hbar}[E_{\vec p}t - \vec p\cdot\vec r]} = u\, e^{-\frac{i}{\hbar}[E_{\vec p}t - \vec p\cdot\vec r]}$$

which are solutions of $H\psi_{\vec p} = E_{\vec p}\psi_{\vec p}$, i.e.

$$(c\,\vec\alpha\cdot\vec p + \beta mc^2)u = \begin{pmatrix} 0 & c\vec\sigma\cdot\vec p \\ c\vec\sigma\cdot\vec p & 0 \end{pmatrix} u +$$

$$+ \begin{pmatrix} mc^2 & 0 & 0 & 0 \\ 0 & mc^2 & 0 & 0 \\ 0 & 0 & -mc^2 & 0 \\ 0 & 0 & 0 & -mc^2 \end{pmatrix} u = E_{\vec p} u$$

a) Particle at rest

For $\vec p = 0$ the problem is diagonal and the solutions are

$$\left.\begin{array}{l} u_+^{(1)} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix},\quad u_+^{(2)} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \quad \text{with } E_0 = mc^2 > 0 \\[2em] u_-^{(1)} = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix},\quad u_-^{(2)} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \quad \text{with } E_0 = -mc^2 < 0 \end{array}\right\}$$

b) Spin

What is the difference between the two solutions $u^{(1)}, u^{(2)}$ for positive and negative energies?

To see this we introduce the operator

$$\vec{\Sigma} = \begin{pmatrix} \vec{\sigma} & 0 \\ 0 & \vec{\sigma} \end{pmatrix} = (\Sigma^1, \Sigma^2, \Sigma^3)$$

and note that $\vec{\Sigma}\cdot\vec{p}$ commutes with H because

$$\begin{pmatrix} 0 & \vec{\sigma}\cdot\vec{p} \\ \vec{\sigma}\cdot\vec{p} & 0 \end{pmatrix}\begin{pmatrix} \vec{\sigma}\cdot\vec{p} & 0 \\ 0 & \vec{\sigma}\cdot\vec{p} \end{pmatrix} = \begin{pmatrix} 0 & (\vec{\sigma}\cdot\vec{p})^2 \\ (\vec{\sigma}\cdot\vec{p})^2 & 0 \end{pmatrix} =$$

$$= \begin{pmatrix} \vec{\sigma}\cdot\vec{p} & 0 \\ 0 & \vec{\sigma}\cdot\vec{p} \end{pmatrix}\begin{pmatrix} 0 & \vec{\sigma}\cdot\vec{p} \\ \vec{\sigma}\cdot\vec{p} & 0 \end{pmatrix}.$$

Thus $\vec{\Sigma}\cdot\vec{p}$ is a conserved quantity associated with the particle spin

$$\vec{S} = \frac{1}{2}\hbar\vec{\Sigma}$$

The spin component in the direction of $\vec{p}$ defines the helicity of the particle and is conserved. The other spin components are not conserved, because angular momentum conservation holds only for the total angular momentum

$$\vec{J} = \vec{L} + \frac{1}{2}\hbar\vec{\Sigma} = \vec{L} + \vec{S}$$ exercise

Obviously $\vec{L}\cdot\vec{p} = 0$, and therefore $\vec{S}\cdot\vec{p}$ is conserved.

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c) Solution of the eigenvalue problem

For a particle moving in the z-direction, $\vec{p} = (0, 0, p)$, the eigenvalue problem reads

$$\begin{pmatrix} mc^2 & 0 & cp & 0 \\ 0 & mc^2 & 0 & -cp \\ -cp & 0 & -mc^2 & 0 \\ 0 & -cp & 0 & -mc^2 \end{pmatrix}\begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{pmatrix} = E_{\vec{p}}\begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{pmatrix}$$

because $\sigma^3 = \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$.

This decouples into separate 2×2 eigenvalue problems for (u_1, u_3) and (u_2, u_4), respectively:

$$\begin{pmatrix} mc^2 & cp \\ cp & -mc^2 \end{pmatrix} \begin{pmatrix} u_1 \\ u_3 \end{pmatrix} = E_{\vec{p}} \begin{pmatrix} u_1 \\ u_3 \end{pmatrix}$$

The eigenvalues are solution of

$$\left.\begin{aligned} &(mc^2 - E_{\vec{p}})(-mc^2 - E_{\vec{p}}) - c^2p^2 = 0 \\ &\Rightarrow \quad \underline{E_{\vec{p}}^2 = c^2p^2 + (mc^2)^2} \end{aligned}\right\} \text{ as expected}$$

The eigenvector components satisfy

$$\underline{u_1 = \frac{cp}{E_{\vec{p}} - mc^2}\, u_3}\,, \quad \underline{u_3 = \frac{cp}{E_{\vec{p}} + mc^2}\, u_1}$$

Two cases:

(i) $\underline{E_{\vec{p}} > 0}$: We set $u_1 = 1$ and use

$$u_3 = \frac{cp}{E_{\vec{p}} + mc^2} \simeq \begin{cases} cp/2mc^2 \ll 1 & p \to 0 \\ 1 & p \to \infty \end{cases}$$

$$\Rightarrow \underline{u_+^{(1)}(\vec{p}) = \begin{pmatrix} 1 \\ 0 \\ \dfrac{cp}{E_{\vec{p}} + mc^2} \\ 0 \end{pmatrix}}$$

converges to the $\vec{p} = 0$ solution derived previously

(ii) $\underline{E_{\vec{p}} < 0}$: Now we set $u_3 = 1$ and use

$$u_1 = \frac{cp}{E_{\vec{p}} - mc^2} = \frac{cp}{-(|E_{\vec{p}}| + mc^2)} \simeq \begin{cases} -\,cp/2mc^2 \,, & p \to 0 \\ -1 \,, & p \to \infty \end{cases}$$

$$\Rightarrow \quad u_-^{(1)}(\vec{p}) = \begin{pmatrix} -\dfrac{cp}{|E_{\vec{p}}| + mc^2} \\ 0 \\ 1 \\ 0 \end{pmatrix}$$

converges to $u_-^{(1)}$ for $p \to 0$

The solution of the eigenvalue problem for u_2, u_4 leads to the remaining two eigenstates

$$u_+^{(2)}(\vec{p}) = \begin{pmatrix} 0 \\ 1 \\ 0 \\ -\dfrac{cp}{E_{\vec{p}} + mc^2} \end{pmatrix} \qquad \underline{E_{\vec{p}} > 0}$$

$$u_-^{(2)}(\vec{p}) = \begin{pmatrix} 0 \\ \dfrac{cp}{|E_{\vec{p}}| + mc^2} \\ 0 \\ 1 \end{pmatrix} \qquad \underline{E_{\vec{p}} < 0}$$

The helicity operator

$$\Sigma^3 = \begin{pmatrix} \sigma^3 & 0 \\ 0 & \sigma^3 \end{pmatrix} = \begin{pmatrix} 1 & & & 0 \\ & -1 & & \\ & & 1 & \\ 0 & & & -1 \end{pmatrix}$$

acts on these eigenstates according to

$$\left.\begin{aligned} \Sigma^3 u_+^{(1)} &= u_+^{(1)}, \quad \Sigma^3 u_-^{(1)} = u_-^{(1)} \\ \Sigma^3 u_+^{(2)} &= -u_+^{(2)}, \quad \Sigma^3 u_-^{(2)} = -u_-^{(2)} \end{aligned}\right\}$$

Hence $u^{(1)}$ and $u^{(2)}$ are states of positive and negative helicity, respectively:

$$\left.\begin{aligned} u_{+,-}^{(1)} &=: u_{+,-}^{\uparrow} \quad \text{"spin up"} \\ u_{+,-}^{(2)} &=: u_{+,-}^{\downarrow} \quad \text{"spin down"} \end{aligned}\right\}$$

Summary:

(i) The 4 components of the Dirac spinor describe solutions with positive and negative energy and positive and negative helicity (spin), respectively.

(ii) In the non-relativistic (low energy) limit

$$\frac{cp}{mc^2} \simeq \frac{v}{c} \ll 1 \qquad (p \simeq mv)$$

the positive energy solution has most weight in the upper components u_1, u_2, the negative energy solution in the lower components u_3, u_4.
At high energies ($p \to \infty$) the upper and lower components have equal weight.

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d) Interpretation of the negative energy solutions

- Negative energy states are problematic because they can be reached from positive energy states by spontaneous emission, i.e. the particles in the positive energy states are unstable.

- Dirac solves this problem by appealing to the Pauli principle for fermions:

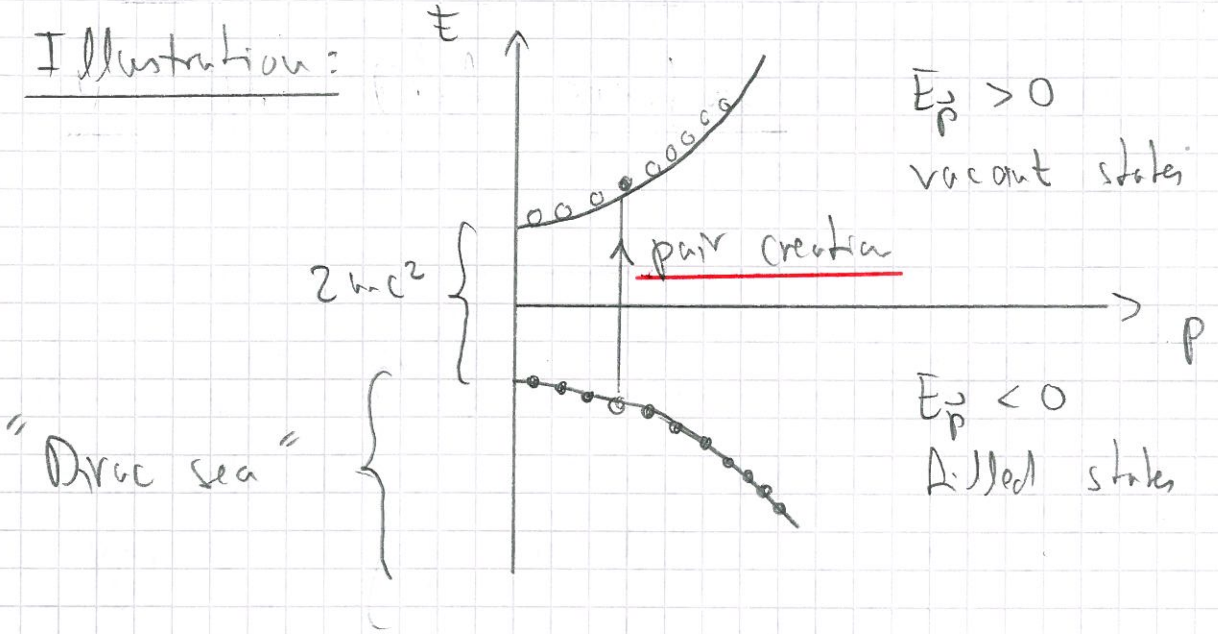
  (i) If all negative energy states are already filled, transition from positive energy states cannot occur.

  (ii) A vacant negative energy state ("hole") would appear as a particle with positive energy but charge opposite to that of "normal" particles

$\Rightarrow$ Dirac equation predicts the existence of antiparticles; positron is discovered in 1933.

- This argument cannot be applied to the solutions of the Klein-Gordon equation, which are spinless and hence bosons.

Illustration:



Remarks:
- The picture is analogous to the free electron gas in solid state theory
- The electrons in the Dirac sea are generally unobservable, similar to the vacuum energy of the electromagnetic field, but phenomena of quantum electrodynamics such as vacuum polarization can be attributed to their existence.

4° The Pauli equation

<u>Goal:</u> Describe the interaction of the Dirac particle with a (classical) electromagnetic field, in the <u>low energy limit</u>.

The electromagnetic field is introduced as in IV. 3°:

$$H = c\vec{\alpha}\cdot\vec{p} + \beta mc^2 \longrightarrow c\vec{\alpha}\cdot\underbrace{(\vec{p} - \tfrac{e}{c}\vec{A})}_{=:\vec{\pi}} + \beta mc^2 + e\Phi$$

$$\begin{cases} \vec{A} : & \text{vector potential} \\ \Phi : & \text{scalar potential} \end{cases}$$

To separate out the low-energy behavior we write the wave function in terms of two 2-spinors:

$$\psi = \begin{pmatrix} \tilde{\varphi} \\ \tilde{\chi} \end{pmatrix}, \quad \tilde{\varphi} = \begin{pmatrix} \tilde{\varphi}_1 \\ \tilde{\varphi}_2 \end{pmatrix} \quad \text{upper component}$$

$$\tilde{\chi} = \begin{pmatrix} \tilde{\chi}_1 \\ \tilde{\chi}_2 \end{pmatrix} \quad \text{lower component}$$

Using that $\vec{\alpha} = \begin{pmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & \vec{0} \end{pmatrix}$, $\beta = \begin{pmatrix} \mathbb{1}_2 & 0 \\ 0 & -\mathbb{1}_2 \end{pmatrix}$

it follows that $\tilde{\varphi}, \tilde{\chi}$ satisfy

$$i\hbar \begin{pmatrix} \dot{\tilde{\varphi}} \\ \dot{\tilde{\chi}} \end{pmatrix} = \begin{pmatrix} (c\,\vec{\sigma}\cdot\vec{\pi})\tilde{\chi} \\ (c\,\vec{\sigma}\cdot\vec{\pi})\tilde{\varphi} \end{pmatrix} + mc^2 \begin{pmatrix} \tilde{\varphi} \\ -\tilde{\chi} \end{pmatrix} + \begin{pmatrix} \tilde{\varphi} \\ \tilde{\chi} \end{pmatrix} e\Phi$$

In the non-relativistic regime, the rest energy mc^2 is the largest energy by far. We eliminate the corresponding term from the equation for $\tilde{\Phi}$ by making the ansatz

$$\begin{pmatrix} \tilde{\varphi} \\ \tilde{\chi} \end{pmatrix} = e^{-\frac{i}{\hbar} mc^2 t} \begin{pmatrix} \varphi \\ \chi \end{pmatrix} \qquad (*)$$

where φ, χ are assumed to vary much more slowly than $\exp(-\frac{i}{\hbar} mc^2 t)$. The resulting equations are

$$\left.\begin{aligned} i\hbar \frac{\partial \varphi}{\partial t} &= c(\vec{\sigma}\cdot\vec{\pi})\chi + e\Phi\varphi \\ i\hbar \frac{\partial \chi}{\partial t} &= \underbrace{c(\vec{\sigma}\cdot\vec{\pi})\varphi - 2mc^2\chi}_{} + e\Phi\chi \end{aligned}\right\}$$

dominant terms, because mc^2 is the largest energy scale and because we expect $|\varphi| \gg |\chi|$ in the non-relativistic limit; more precisely, we expect $|\chi|/|\varphi| \simeq v/c = p/mc^2$

Thus the equation for χ is approximately solved by

$$\chi = \frac{1}{2mc}(\vec{\sigma}\cdot\vec{\pi})\varphi$$

Remark: The transformation (*) amounts to shifting the zero of the energy scale to the rest energy mc^2.

Inserting χ into the equation for φ we have

$$i\hbar \frac{\partial \varphi}{\partial t} = \frac{1}{2m} (\vec{\sigma} \cdot \vec{\pi})^2 \varphi + e \Phi \varphi$$

To evaluate the kinetic energy term we make use of the identity

$$(\vec{\sigma} \cdot \vec{a})(\vec{\sigma} \cdot \vec{b}) = \vec{a} \cdot \vec{b} + i \vec{\sigma} \cdot (\vec{a} \times \vec{b})$$

that holds for arbitrary vectors $\vec{a}, \vec{b}$.
In the present case this implies

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

$$\vec{\pi}^2 = \left(\vec{p} - \frac{e}{c} \vec{A}\right)^2$$

$$\vec{\pi} \times \vec{\pi} = \left(-i\hbar \nabla - \frac{e}{c} \vec{A}\right) \times \left(-i\hbar \nabla - \frac{e}{c} \vec{A}\right)$$

$$\frac{i\hbar e}{c} \left[\nabla \times \vec{A} + \vec{A} \times \nabla \right]$$

which acts as an operator on the components of the wave function. Since

$$\nabla \times (\vec{A} f(\vec{r})) = f(\vec{r})(\nabla \times \vec{A}) + (\nabla f) \times \vec{A}$$

$$= f(\vec{r})(\nabla \times \vec{A}) - (\vec{A} \times \nabla) f$$

it follows that

$$\vec{\pi} \times \vec{\pi} = \frac{i\hbar e}{c} (\vec{\nabla} \times \vec{A}) = \frac{i\hbar e}{c} \vec{B}$$

$$\Rightarrow \quad i\hbar \frac{\partial \varphi}{\partial t} = \left[\frac{1}{2m} \left(\vec{p} - \frac{e}{c} \vec{A} \right)^2 - \frac{\hbar e}{2mc} \vec{B} \cdot \vec{\sigma} + e\Phi \right] \varphi$$

Pauli equation

The contribution from the spin can be written as $\vec{B} \cdot \vec{\mu}$, where the magnetic moment of the electron is

$$\vec{\mu} = \frac{\hbar e}{2mc} \vec{\sigma}$$

Since the corresponding angular momentum is $\vec{S} = \frac{\hbar}{2} \vec{\sigma}$, we can write

$$\vec{\mu} = \underbrace{\frac{e}{mc}}_{\text{gyromagnetic ratio}} \vec{S}$$

This is twice the value $\frac{e}{2mc}$ expected for a rotating charge distribution

$\Rightarrow$ the gyromagnetic factor of the Dirac electron is $g = 2$.