3.8 Nonrelativistic limit of the free Dirac equation

- Dirac equation in non-covariant form:
  \[ i\hbar \frac{\partial}{\partial t} \psi = \left( \frac{\hbar c}{i} \vec{\alpha} \cdot \vec{\nabla} + \beta mc^2 \right) \psi \]

- Solutions with positive energy and \( \vec{p} = 0 \):
  \[ \psi = u_s(\vec{p} = 0) e^{-\frac{i}{\hbar}mc^2 t} \]

- Small nonvanishing momenta:
  \[ \vec{p}^2 \ll mc^2 \]

  \[ \Rightarrow E - mc^2 \approx \frac{\vec{p}^2}{2m} \ll mc^2 \quad \rightarrow \quad \text{ansatz:} \quad \psi(t, \vec{x}) = e^{-\frac{i}{\hbar}mc^2 t} \begin{pmatrix} \varphi(t, \vec{x}) \\ \chi(t, \vec{x}) \end{pmatrix} \]

- \( \varphi, \chi \): two-component spinors, only slowly varying in time in comparison with \( e^{-\frac{i}{\hbar}mc^2 t} \):

  \[ |i\hbar \frac{\partial}{\partial t} \varphi| \ll |mc^2 \varphi|, \quad |i\hbar \frac{\partial}{\partial t} \chi| \ll |mc^2 \chi| \]
\[
\psi(t, \vec{x}) = e^{-\frac{i}{\hbar} mc^2 t} \begin{pmatrix} \varphi(t, \vec{x}) \\ \chi(t, \vec{x}) \end{pmatrix}
\]

\[
\Rightarrow \quad i\hbar \frac{\partial}{\partial t} \psi = \begin{pmatrix} mc^2 \varphi + i\hbar \frac{\partial \varphi}{\partial t} \\ mc^2 \chi + i\hbar \frac{\partial \chi}{\partial t} \end{pmatrix} e^{-\frac{i}{\hbar} mc^2 t}
\]

\[
= \left( \frac{\hbar c}{i} \vec{\alpha} \cdot \vec{\nabla} + \beta mc^2 \right) \psi = \begin{pmatrix} \frac{\hbar c}{i} \begin{pmatrix} 0 & \vec{\sigma} \cdot \vec{\nabla} \\ \vec{\sigma} \cdot \vec{\nabla} & 0 \end{pmatrix} + \begin{pmatrix} mc^2 & 0 \\ 0 & -mc^2 \end{pmatrix} \end{pmatrix} \psi
\]

\[
= \begin{pmatrix} mc^2 \varphi + \frac{\hbar c}{i} \vec{\sigma} \cdot \vec{\nabla} \chi \\ -mc^2 \chi + \frac{\hbar c}{i} \vec{\sigma} \cdot \vec{\nabla} \varphi \end{pmatrix} e^{-\frac{i}{\hbar} mc^2 t}
\]

\[
\Rightarrow \quad i\hbar \frac{\partial \varphi}{\partial t} = \frac{\hbar c}{i} \vec{\sigma} \cdot \vec{\nabla} \chi
\]

\[
i\hbar \frac{\partial \chi}{\partial t} = \frac{\hbar c}{i} \vec{\sigma} \cdot \vec{\nabla} \varphi - 2mc^2 \chi
\]
\[
\psi(t, \vec{x}) = e^{-\frac{i}{\hbar} mc^2 t} \begin{pmatrix} \varphi(t, \vec{x}) \\ \chi(t, \vec{x}) \end{pmatrix}
\]

\[
\Rightarrow \quad i\hbar \frac{\partial}{\partial t} \psi = \begin{pmatrix} mc^2 \varphi + i\hbar \frac{\partial \varphi}{\partial t} \\ mc^2 \chi + i\hbar \frac{\partial \chi}{\partial t} \end{pmatrix} e^{-\frac{i}{\hbar} mc^2 t}
\]

\[
= \left( \frac{\hbar}{i} \vec{\alpha} \cdot \nabla + \beta mc^2 \right) \psi = \left[ \frac{\hbar}{i} \begin{pmatrix} 0 & \vec{\sigma} \cdot \nabla \\ \vec{\sigma} \cdot \nabla & 0 \end{pmatrix} \right] + \left( \begin{pmatrix} mc^2 & 0 \\ 0 & -mc^2 \end{pmatrix} \right) \psi
\]

\[
= \begin{pmatrix} mc^2 \varphi + \frac{\hbar c}{i} \vec{\sigma} \cdot \nabla \chi \\ -mc^2 \chi + \frac{\hbar c}{i} \vec{\sigma} \cdot \nabla \varphi \end{pmatrix} e^{-\frac{i}{\hbar} mc^2 t}
\]

\[
\Rightarrow \quad i\hbar \frac{\partial \varphi}{\partial t} = \frac{\hbar c}{i} \vec{\sigma} \cdot \nabla \chi
\]

\[
i\hbar \frac{\partial \chi}{\partial t} = \frac{\hbar c}{i} \vec{\sigma} \cdot \nabla \varphi - 2mc^2 \chi \quad |i\hbar \frac{\partial \chi}{\partial t}| \ll |mc^2 \chi| \quad \chi \approx \frac{\hbar}{2imc} \vec{\sigma} \cdot \nabla \varphi
\]
\[ \psi(t, \vec{x}) = e^{-\frac{i}{\hbar}mc^2 t} \begin{pmatrix} \varphi(t, \vec{x}) \\ \chi(t, \vec{x}) \end{pmatrix} \]

\[ \Rightarrow \quad i\hbar \frac{\partial}{\partial t} \psi = \begin{pmatrix} mc^2 \varphi + i\hbar \frac{\partial \varphi}{\partial t} \\ mc^2 \chi + i\hbar \frac{\partial \chi}{\partial t} \end{pmatrix} e^{-\frac{i}{\hbar}mc^2 t} \]

\[ = \begin{pmatrix} \frac{\hbar c}{i} \vec{\alpha} \cdot \vec{\nabla} + \beta mc^2 \end{pmatrix} \psi = \begin{pmatrix} \frac{\hbar c}{i} \begin{pmatrix} 0 & \vec{\sigma} \cdot \vec{\nabla} \\ \vec{\sigma} \cdot \vec{\nabla} & 0 \end{pmatrix} + \begin{pmatrix} mc^2 & 0 \\ 0 & -mc^2 \end{pmatrix} \end{pmatrix} \psi \]

\[ = \begin{pmatrix} mc^2 \varphi + \frac{\hbar c}{i} \vec{\sigma} \cdot \vec{\nabla} \chi \\ -mc^2 \chi + \frac{\hbar c}{i} \vec{\sigma} \cdot \vec{\nabla} \varphi \end{pmatrix} e^{-\frac{i}{\hbar}mc^2 t} \]

\[ \Rightarrow \quad i\hbar \frac{\partial \varphi}{\partial t} = \frac{\hbar c}{i} \vec{\sigma} \cdot \vec{\nabla} \chi \quad \Rightarrow \quad i\hbar \frac{\partial \varphi}{\partial t} \approx -\frac{\hbar^2}{2m} (\vec{\sigma} \cdot \vec{\nabla})^2 \varphi \]

\[ i\hbar \frac{\partial \chi}{\partial t} = \frac{\hbar c}{i} \vec{\sigma} \cdot \vec{\nabla} \varphi - 2mc^2 \chi \quad |i\hbar \frac{\partial \chi}{\partial t}| \ll |mc^2 \chi| \quad \Rightarrow \quad \chi \approx \frac{\hbar}{2imc} \vec{\sigma} \cdot \vec{\nabla} \varphi \]
\[ i\hbar \frac{\partial \varphi}{\partial t} \approx -\frac{\hbar^2}{2m} (\vec{\sigma} \cdot \vec{\nabla})^2 \varphi \]

- reminder: \( (\vec{\sigma} \cdot \vec{a})(\vec{\sigma} \cdot \vec{b}) = \vec{a} \cdot \vec{b} + i(\vec{a} \times \vec{b}) \cdot \vec{\sigma} \)

\[ \Rightarrow \quad i\hbar \frac{\partial}{\partial t} \varphi \approx -\frac{\hbar^2}{2m} \vec{\nabla}^2 \varphi \]

- Schrödinger-like equation for the two-component spinor \( \varphi \)
  (\( \rightarrow \) Pauli spinor, spin \( \frac{1}{2} \), see later)

- plane waves: \( \varphi \propto e^{-\frac{i}{\hbar}(E_{nr}t - \vec{p} \cdot \vec{x})} \), \( E_{nr} = \frac{\vec{p}^2}{2m} \)

\[ \Rightarrow \quad \chi \approx \frac{\hbar}{2imc} \vec{\sigma} \cdot \vec{\nabla} \varphi = \frac{\vec{\sigma} \cdot \vec{p}}{2mc} \varphi \quad |\vec{p}| \ll mc \quad |\chi| \ll |\varphi| \]

- sensible non-relativistic limit
3.9 Dirac equation with elektromagnetic field

- minimal substitution: \( \partial_\mu \rightarrow D_\mu = \partial_\mu + \frac{iq}{\hbar c} A_\mu \)

insert into the free Dirac equation:

\[
\Rightarrow \left( i \frac{\partial}{\partial t} - \frac{mc}{\hbar} \right) \psi = \left( i \frac{\partial}{\partial t} - \frac{q}{\hbar c} \vec{A} - \frac{mc}{\hbar} \right) \psi = 0
\]

- non-covariant form:

\[
i\hbar \frac{\partial}{\partial t} \rightarrow i\hbar \frac{\partial}{\partial t} - q\phi, \quad \frac{\hbar}{i} \vec{\nabla} \rightarrow \frac{\hbar}{i} \vec{\nabla} - \frac{q}{c} \vec{A}
\]

\[
\Rightarrow \left( i\hbar \frac{\partial}{\partial t} - q\phi \right) \psi = \left[ \vec{\alpha} \cdot \frac{\hbar c}{i} \left( \vec{\nabla} - \frac{iq}{\hbar c} \vec{A} \right) + \beta mc^2 \right] \psi
\]

\[
\Leftrightarrow i\hbar \frac{\partial}{\partial t} \psi = \left[ \vec{\alpha} \cdot \frac{\hbar c}{i} \left( \vec{\nabla} - \frac{iq}{\hbar c} \vec{A} \right) + \beta mc^2 + q\phi \right] \psi
\]
\[ i\hbar \frac{\partial}{\partial t} \psi = \left[ \vec{\alpha} \cdot \frac{\hbar c}{i} (\vec{\nabla} - \frac{iq}{\hbar c} \vec{A}) + \beta mc^2 + q\phi \right] \psi \]

- nonrelativistic approximation + weak electric fields: \( |\vec{p}|c, q\phi \ll mc^2 \)

\[ \rightarrow \text{ansatz as before: } \psi = \begin{pmatrix} \varphi \\ \chi \end{pmatrix} e^{-\frac{i}{\hbar}mc^2 t} \]

\[ \Rightarrow i\hbar \frac{\partial}{\partial t} \varphi = \left[ -\frac{\hbar^2}{2m} \vec{\sigma} \cdot (\vec{\nabla} - \frac{iq}{\hbar c} \vec{A}) \vec{\sigma} \cdot (\vec{\nabla} - \frac{iq}{\hbar c} \vec{A}) + q\phi \right] \varphi \]

exercises

\[ i\hbar \frac{\partial}{\partial t} \varphi = \left[ -\frac{\hbar^2}{2m} \left(\vec{\nabla} - \frac{iq}{\hbar c} \vec{A}\right)^2 - \frac{\hbar q}{2mc} \vec{\sigma} \cdot \vec{B} + q\phi \right] \varphi \quad (\vec{B} = \vec{\nabla} \times \vec{A}) \]

Pauli equation for nonrelativistic spin-\( \frac{1}{2} \) particles in an electromagnetic field
Simplifications:

- homogeneous magnetic field: $\vec{B} = \text{const.}$
  (e.g., choose $\vec{A} = \frac{1}{2} \vec{B} \times \vec{x}$)

- weak magnetic field: neglect $\vec{B}^2$ terms

Exercises

$$i\hbar \frac{\partial}{\partial t} \varphi = \left[ -\frac{\hbar^2}{2m} \vec{\nabla}^2 - \frac{q}{2mc} \left( \vec{L} + 2\vec{S} \right) \cdot \vec{B} + q \phi \right] \varphi$$

with $\vec{L} = \vec{x} \times \vec{p} = \vec{x} \times \frac{\hbar}{i} \vec{\nabla}$ orbital angular momentum

$\vec{S} = \frac{\hbar}{2} \vec{\sigma}$ spin
Spin

- Reminder of nonrelativistic quantum mechanics:

\[ \vec{S} = \frac{\hbar}{2} \vec{\sigma} \Rightarrow S_z = \frac{\hbar}{2} \sigma_3 = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \]

\[ \vec{S}^2 = \frac{\hbar^2}{4} (\sigma_1^2 + \sigma_2^2 + \sigma_3^2) = \frac{3}{4} \hbar^2 \mathbb{1} = s(s + 1)\hbar^2 \mathbb{1} \quad \text{with} \quad s = \frac{1}{2} \]

- simultaneous eigenstates of \( \vec{S}^2 \) and \( S_z \):

\[ |s = \frac{1}{2}, m_s = +\frac{1}{2}\rangle \equiv \varphi_\uparrow \equiv \begin{pmatrix} 1 \\ 0 \end{pmatrix} \Rightarrow S_z \varphi_\uparrow = \frac{\hbar}{2} \varphi_\uparrow \]

\[ |s = \frac{1}{2}, m_s = -\frac{1}{2}\rangle \equiv \varphi_\downarrow \equiv \begin{pmatrix} 0 \\ 1 \end{pmatrix} \Rightarrow S_z \varphi_\downarrow = -\frac{\hbar}{2} \varphi_\downarrow \]
We had: 

\[ i\hbar \frac{\partial}{\partial t} \varphi = \left[ -\frac{\hbar^2}{2m} \nabla^2 - \frac{q}{2mc} \left( \vec{L} + 2\vec{S} \right) \cdot \vec{B} + q\phi \right] \varphi \]

→ magnetic interaction energy:

\[ E_{\text{magn}} = -\frac{q}{2mc} \left( \vec{L} + 2\vec{S} \right) \cdot \vec{B} \equiv -\vec{\mu} \cdot \vec{B} \]

→ magnetic moment: 

\[ \vec{\mu} = \vec{\mu}_{\text{orb}} + \vec{\mu}_{\text{spin}} \]

- \[ \vec{\mu}_{\text{orb}} = \frac{q}{2mc} \vec{L} \]

- \[ \vec{\mu}_{\text{spin}} = \frac{q}{2mc} 2\vec{S} \equiv \frac{q}{2mc} g\vec{S}, \quad g = 2 \quad \text{“gyromagnetic ratio”} \]

→ experimental value: 

\[ g_{e^-} = 2 \cdot (1.001 159 652 180 73(28)) \]

↑ QED corrections

\[ g_p = 2 \cdot 2.79 \quad \text{not a pointlike “Dirac particle”} \]
3.10 Interpretation of the solutions with negative energy

Instability problem: An electron could lower its energy further and further by emitting photons. (all figures in this section in “natural units”: \( c = 1 \))

⇒ All atoms would be unstable (live time \( \tau = 0 \))!
3.10 Interpretation of the solutions with negative energy

- Instability problem:

\[ E = \sqrt{\vec{p}^2 + m^2} \]

An electron could lower its energy further and further by emitting photons.

\[ E = -\sqrt{\vec{p}^2 + m^2} \]

(all figures in this section in “natural units”: \( c = 1 \))
3.10 Interpretation of the solutions with negative energy

- Instability problem:

An electron could lower its energy further and further by emitting photons.

(all figures in this section in “natural units”: c = 1)
3.10 Interpretation of the solutions with negative energy

- Instability problem:

\[ E = \pm \sqrt{p^2 + m^2} \]

An electron could lower its energy further and further by emitting photons.

(all figures in this section in “natural units”: \( c = 1 \))

⇒ All atoms would be unstable (live time \( \tau = 0 \))!
Dirac’s solution: “hole theory”

- physical vacuum (“Dirac sea”):
  - states with $E > 0$ empty
  - states with $E < 0$ occupied

Transitions of additional $E > 0$ fermions into negative-energy states Pauli forbidden!

Energy and charge of the vacuum = $-\infty$ (for electrons)

“renormalization”: Energy and charge are measured relative to the occupied Dirac sea.
Dirac’s solution: “hole theory”

- physical vacuum (“Dirac sea”):
  - states with $E > 0$ empty
  - states with $E < 0$ occupied

$\Rightarrow$ Transitions of additional $E > 0$ fermions into negative-energy states Pauli forbidden!
Dirac’s solution: “hole theory”

- physical vacuum ("Dirac sea"):
  - states with $E > 0$ empty
  - states with $E < 0$ occupied

⇒ Transitions of additional $E > 0$ fermions into negative-energy states Pauli forbidden!

- occupied Dirac sea:
  - energy and charge of the vacuum = $-\infty$ (for electrons)
Dirac’s solution: “hole theory”

- physical vacuum (“Dirac sea”):
  - states with $E > 0$ empty
  - states with $E < 0$ occupied

$\Rightarrow$ Transitions of additional $E > 0$ fermions into negative-energy states Pauli forbidden!

- occupied Dirac sea:
  - energy and charge of the vacuum = $-\infty$ (for electrons)
  - “renormalization”:
    Energy and charge are measured relative to the occupied Dirac sea.
Consequence:

Adding an amount of energy $\Delta E > 2mc^2$ to the system (e.g., by radiation), an electron in the Dirac sea can be lifted into a positive-energy state:

Creation of a “particle” with energy $E > 0$ and a “hole” in the Dirac sea
Consequence:

Adding an amount of energy $\Delta E > 2mc^2$ to the system (e.g., by radiation), an electron in the Dirac sea can be lifted into a positive-energy state:

Creation of a “particle” with energy $E > 0$ and a “hole” in the Dirac sea

Interpretation of the holes:

missing particle with energy $E_h < 0$, momentum $\vec{p}_h$, spin $s_h$, charge $q_h$, ...

= antiparticle w/ energy $-E_h > 0$, momentum $-\vec{p}_h$, spin $-s_h$, charge $-q_h$, ...
Consequence:

Adding an amount of energy $\Delta E > 2mc^2$ to the system (e.g., by radiation), an electron in the Dirac sea can be lifted into a positive-energy state:

Creation of a “particle” with energy $E > 0$ and a “hole” in the Dirac sea

Interpretation of the holes:

missing particle with energy $E_h < 0$, momentum $\vec{p}_h$, spin $s_h$, charge $q_h$, ...

= antiparticle w/ energy $-E_h > 0$, momentum $-\vec{p}_h$, spin $-s_h$, charge $-q_h$, ...

→ pair creation: $\gamma^* \rightarrow e^+ e^-$
Consequence:

Adding an amount of energy $\Delta E > 2mc^2$ to the system (e.g., by radiation), an electron in the Dirac sea can be lifted into a positive-energy state:

Creation of a “particle” with energy $E > 0$ and a “hole” in the Dirac sea

Interpretation of the holes:

missing particle with energy $E_h < 0$, momentum $\vec{p}_h$, spin $s_h$, charge $q_h$, ...

= antiparticle w/ energy $-E_h > 0$, momentum $-\vec{p}_h$, spin $-s_h$, charge $-q_h$, ...

→ pair creation: $\gamma^* \rightarrow e^+ e^-$

inverse reaction: $e^+ e^- \rightarrow \gamma^*$ (pair annihilation)
recombination of particle and hole
most spectacular success:
Based on these considerations Dirac predicted the positron before its detection by Anderson 1932.
Discussion

- most spectacular success:
  Based on these considerations Dirac predicted the positron before its detection by Anderson 1932.

- problems:
  - conceptionally: The hole theory does not work for bosons.
**Discussion**

- **most spectacular success:**
  Based on these considerations Dirac predicted the positron before its detection by Anderson 1932.

- **problems:**
  - conceptionally: The hole theory does not work for bosons.
  - technically: It is unavoidably an infinite many-body theory.
Discussion

- **most spectacular success:**
  Based on these considerations Dirac predicted the positron before its detection by Anderson 1932.

- **problems:**
  - conceptionally: The hole theory does not work for bosons.
  - technically: It is unavoidably an infinite many-body theory.

- **modern perspective:**
  - The boson problem is solved within quantum field theory, which makes the hole theory obsolet for fermions as well.
Discussion

- most spectacular success:
  Based on these considerations Dirac predicted the positron before its detection by Anderson 1932.

- problems:
  - conceptionally: The hole theory does not work for bosons.
  - technically: It is unavoidably an infinite many-body theory.

- modern perspective:
  - The boson problem is solved within quantum field theory, which makes the hole theory obsolet for fermions as well.
  - However, the QFT vacuum has certain similarities to the Dirac sea. QFT extends this concept in a way that is also applicable for bosons.
Discussion

- **most spectacular success:**
  Based on these considerations Dirac predicted the positron before its detection by Anderson 1932.

- **problems:**
  - conceptionally: The hole theory does not work for bosons.
  - technically: It is unavoidably an infinite many-body theory.

- **modern perspective:**
  - The boson problem is solved within quantum field theory, which makes the hole theory obsolet for fermions as well.
  - However, the QFT vacuum has certain similarities to the Dirac sea. QFT extends this concept in a way that is also applicable for bosons.
  - The infinite many-body problem remains.
The concept of the hole theory is still used in many-body theory, e.g., in condensed-matter physics or nuclear physics. There one considers particle-hole excitations in the Fermi sea, whereas the Dirac sea is often neglected.