VII Relativistic wave equations for spin 1/2 particles: Dirac equation

VII.1 Dirac equation

One problem of the KGE was that there is no positive definite density which would allow for a probability interpretation. This is related to the fact that the KGE is second order in time

Dirac (1928): trial of a 1st order equation

(414) $$i\hbar \frac{\partial}{\partial t}\psi = \frac{\hbar c}{i}\left(\alpha_1 \frac{\partial \psi}{\partial x_1} + \alpha_2 \frac{\partial \psi}{\partial x_2} + \alpha_3 \frac{\partial \psi}{\partial x_3}\right) + \beta m c^2 \psi = H\psi$$

- α_i cannot be c-numbers as then (414) would not be invariant under rotation

$\Rightarrow$ α_i, β $N \times N$ matrices

(415) and $$\psi = \begin{pmatrix} \psi_1 \\ \vdots \\ \psi_N \end{pmatrix}$$ N component vector

condition to this construction

(i) there should be a continuity equation for

$$\varrho(\vec{r},t) = \Psi^{+}(\vec{r},t)\cdot\Psi(\vec{r},t) = \sum_{i=1}^{N} \Psi_i^{*}(\vec{r},t)\Psi_i(\vec{r},t) \geq 0$$

(ii) Lorentz invariance

(iii) for free particles

$$E^2 = \hbar^2\omega^2 \overset{!}{=} \vec{p}^{\,2}c^2 + m_0^2c^4$$

In order to fulfill (iii) every component of Ψ must fulfill KGE

$$-\hbar^2 \frac{\partial^2 \Psi_j}{\partial t^2} \overset{!}{=} \left(-\hbar^2c^2\Delta + m_0^2c^4\right)\Psi_j \qquad (416)$$

$$\forall j = 1,2,\dots N$$

With ansatz (414) one finds

$$-\hbar^2\frac{\partial^2\Psi}{\partial t^2} = -\hbar^2c^2\sum_{k,l=1}^{3}\frac{\alpha_k\alpha_l+\alpha_l\alpha_k}{2}\frac{\partial^2}{\partial x^k\partial x^l}\Psi$$

$$+\frac{\hbar m_0c^3}{i}\sum_{l=1}^{3}\left(\alpha_l\beta+\beta\alpha_l\right)\frac{\partial\Psi}{\partial x^l} + \beta^2m_0^2c^4\Psi$$

comparison with eq. (416) yields

(417) $$\boxed{\alpha_k\alpha_\ell + \alpha_\ell\alpha_k = 2\delta_{\ell k}\,\mathbb{1}}$$

(418) $$\alpha_i\beta + \beta\alpha_i = 0$$

(419) $$\alpha_i^2 = \beta^2 = \mathbb{1}$$

in order for H to be hermitian $H^+ = H$ it follows

(420) $$\boxed{\alpha_i^+ = \alpha_i \qquad \beta_i^+ = \beta}$$

<u>consequences:</u>

(421) • eigenvalues of $\alpha_i, \beta = \pm 1$

(422) • $\mathrm{Tr}\{\alpha_i\} = \mathrm{Tr}\{\beta\} = 0$

since $\alpha_i\beta + \beta\alpha_i = 0 \Rightarrow \alpha_i + \beta\alpha_i\beta = 0$

$$\mathrm{Tr}\{\alpha_i\} = -\mathrm{Tr}\{\beta\alpha_i\beta\} = -\mathrm{Tr}\{\beta^2\alpha_i\}$$
$$= -\mathrm{Tr}\{\alpha_i\} \quad \square$$

$\Rightarrow$ α_i, β are matrices with even dimension

$N=2$ does not work since there are only 3 matrices (Pauli matrices)

$N=4$ minimal dimension

a possible representation of the Dirac matrices

(423) $$\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix} \qquad \beta = \begin{pmatrix} \mathbb{1}_2 & 0 \\ 0 & -\mathbb{1}_2 \end{pmatrix}$$
$i = 1,2,3$

Dirac equation

(424) $$i\hbar \frac{\partial}{\partial t} \psi = \hat{H}\psi \qquad \hat{H} = \left(c\,\underline{\underline{\vec{\alpha}}} \cdot \hat{\vec{p}} + m_0 c^2 \underline{\underline{\beta}}\right)$$

(425) $$\hat{H} = \hat{H}^+ \qquad \psi = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix}$$ bi-spinor

(A) Continuity equation and probability interpretation

We now want to show that one can derive a continuity equation with positive density which allows for a probability interpretation

(426) $$\underbrace{i\hbar\, \psi^+ \partial_t \psi}_{\text{number!}} = \frac{\hbar c}{i} \sum_{k=1}^{3} \psi^+ \alpha_k \partial_k \psi + m_0 c^2 \psi^+ \beta \psi$$

add complex conjugate

$$-i\hbar\left(\partial_t \psi^+\right)\psi = -\frac{\hbar c}{i}\sum_{k=1}^{3}\partial_k \psi^+ \alpha_k \psi + m_0 c^2 \psi^+ \beta \psi$$

$$\Rightarrow$$

$$i\hbar\, \partial_t\left(\psi^+\psi\right) = \frac{\hbar c}{i}\sum_{k=1}^{3}\psi^+ \alpha_k \partial_k \psi + \left(\partial_k \psi^+\right)\alpha_k \psi$$

$$= \frac{\hbar c}{i}\sum_{k=1}^{3}\frac{\partial}{\partial x^k}\left(\psi^+ \alpha_k \psi\right)$$

$$\Rightarrow$$

(427) $$\boxed{\rho \equiv \Psi^+ \Psi = \sum_{k=1}^{4}\psi_i^* \psi_i}$$ probability density

(428) and $$\boxed{j^k = c\, \psi^+ \alpha_k \psi}$$ 3 current density

continuity equation

(429) $$\boxed{\frac{\partial \rho}{\partial t} + \vec{\nabla}\cdot\vec{j} = 0} \quad \text{or} \quad \boxed{\partial_\mu j^\mu = 0}$$

conservation law:

(430) $$\boxed{\frac{d}{dt}\int d^3r\, \Psi^+ \Psi = 0}$$

remark: We still have to show that j^μ transforms like a Lorentz-vector !

(B) free Dirac particle

Let us determine stationary solutions of the Dirac equation

$$i\hbar \frac{\partial}{\partial t} \underline{\Psi} = \hat{H} \underline{\Psi}$$

so

$$\underline{\Psi}(\vec{r},t) = \underline{\Psi}(\vec{r}) e^{-i\varepsilon t/\hbar}$$

$$\Rightarrow \qquad \hat{H} \underline{\Psi}(\vec{r}) = \varepsilon \underline{\Psi}(\vec{r})$$

remember that $\underline{\Psi}$ is a 4 component object

(431) $$\underline{\Psi} = \begin{pmatrix} \varphi \\ \chi \end{pmatrix} \qquad \varphi = \begin{pmatrix} \Psi_1 \\ \Psi_2 \end{pmatrix} \quad \chi = \begin{pmatrix} \Psi_3 \\ \Psi_4 \end{pmatrix}$$

decomposition into two spinors φ, χ.
Substitute into time independent Dirac equation with

$$\hat{H} = c\,\underline{\underline{\vec{\alpha}}} \cdot \hat{\vec{p}} + m_0 c^2 \underline{\beta} \qquad \underline{\vec{\alpha}} = \begin{pmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & 0 \end{pmatrix}$$

yields

(432) $$\varepsilon \begin{pmatrix} \varphi \\ \chi \end{pmatrix} = c \begin{pmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & 0 \end{pmatrix} \cdot \vec{p} \begin{pmatrix} \varphi \\ \chi \end{pmatrix} + m_0 c^2 \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \varphi \\ \chi \end{pmatrix}$$

since obviously $[\hat{H}, \hat{\vec{p}}] = 0 \Rightarrow$

(433) $$\begin{pmatrix} \varphi \\ \chi \end{pmatrix} = \begin{pmatrix} \varphi_0 \\ \chi_0 \end{pmatrix} e^{i\vec{p}\cdot\vec{r}/\hbar} \qquad \vec{p} = \hbar \vec{k}$$

c-number

you will show in the problem course that

$$(434) \quad \boxed{\mathcal{E} = \pm E_p} \qquad \boxed{E_p = \sqrt{c^2p^2 + m_0^2c^4}}$$

and eigensolution

$$(435) \quad \boxed{\chi_0 = \frac{\hbar c\, \vec{\sigma}\cdot\vec{k}}{m_0c^2 + \mathcal{E}}\, \varphi_0}$$

As in the Klein-Gordon theory we find two types of solutions

$$(436) \quad \begin{array}{lll} \mathcal{E} = +E_p & \text{positive frequency} & \text{particle} \\ \mathcal{E} = -E_p & \text{negative frequency} & \text{anti-particle} \end{array}$$

notation $\mathcal{E} = \lambda E_p \qquad \lambda = \pm 1$

$$(437) \quad \boxed{\psi_{\vec{k},\lambda}(\vec{r},t) = \mathcal{N}\begin{pmatrix} \varphi_0 \\ \dfrac{\hbar c\,\vec{\sigma}\cdot\vec{k}}{m_0c^2 + \lambda E_p} \end{pmatrix} \frac{e^{i\left(\vec{k}\cdot\vec{r} - \lambda\frac{E_p t}{\hbar}\right)}}{(2\pi\hbar)^{3/2}}}$$

In order for $\psi_{\vec{k},\lambda}$ to be normalized, i.e.

$$\int d^3r\, \Psi^{\dagger}_{\vec{k},\lambda}(\vec{r},t)\, \Psi_{\vec{k}',\lambda'}(\vec{r},t) \overset{!}{=} \delta_{\lambda\lambda'}\, \delta(\vec{p}-\vec{p}\,')$$

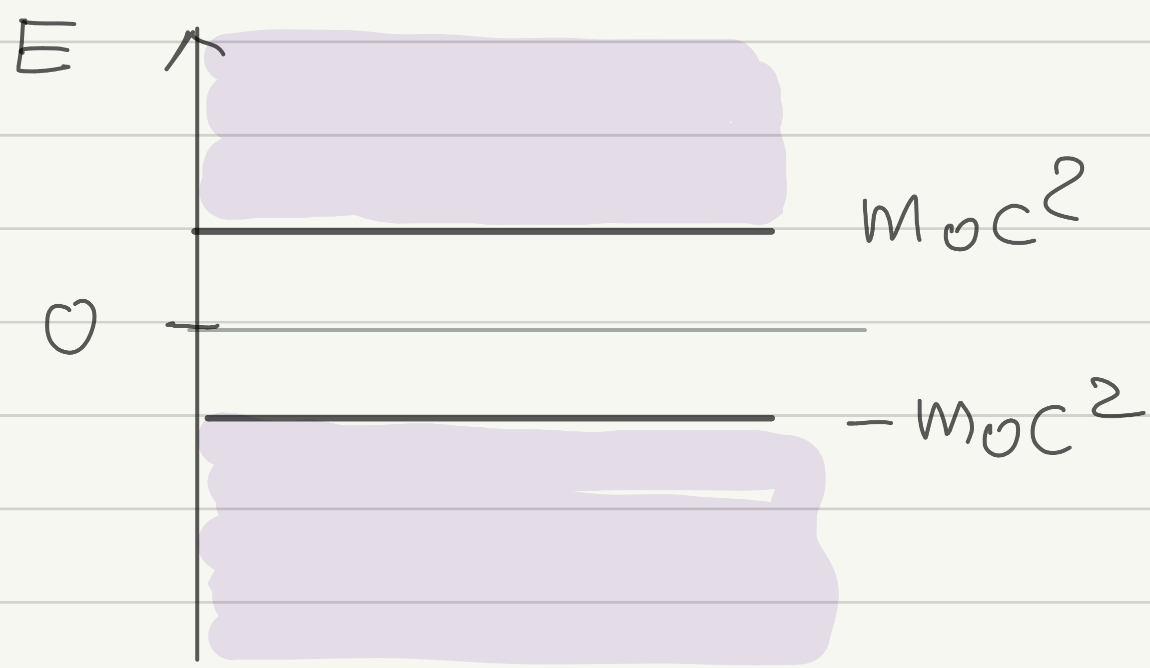
where $\vec{p} = \hbar \vec{k}$ one has

(438) $$\mathcal{N} = \sqrt{\frac{m_0c^2 + \lambda E_p}{2\lambda E_p}}$$

and

(439) $$\varphi_0 = \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} \qquad u_1^* u_1 + u_2^* u_2 = 1$$

Spectrum of free Dirac particle (as for KGE)



The eigenstates (437) for given momentum $\vec{p} = \hbar\vec{k}$ and fixed positive or negative energy i.e. $\lambda = \pm 1$ are still not completely determined

$\longrightarrow$ missing quantum number

▶ helicity

In the problem courses you will show that there is another conserved quantity

(440) $$\boxed{\hat{\vec{S}} \equiv \frac{\hbar}{2}\begin{pmatrix} \hat{\vec{\sigma}} & 0 \\ 0 & \vec{\sigma} \end{pmatrix} \qquad [\hat{\vec{S}}, \hat{H}] = 0}$$

this is the 4-dimensional generalization of the spin

<u>helicity operator</u>: projection of $\vec{S}$ to $\vec{k}$

(441) $$\boxed{\hat{\Lambda}_s \equiv \hat{\vec{S}} \cdot \frac{\vec{k}}{|\vec{k}|} = \hat{\vec{S}} \cdot \frac{\vec{p}}{|\vec{p}|}}$$

- <u>example</u>: $\vec{p} = \hbar\vec{k} = (0, 0, \hbar k)$

(442) $$\hat{\Lambda}_s = \hat{S}_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

eigenvalues: $\lambda = \pm\hbar/2$

(443) eigen vectors $\begin{pmatrix} u_1 \\ 0 \end{pmatrix}, \begin{pmatrix} u_{-1} \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ u_1 \end{pmatrix} \begin{pmatrix} 0 \\ u_{-1} \end{pmatrix}$

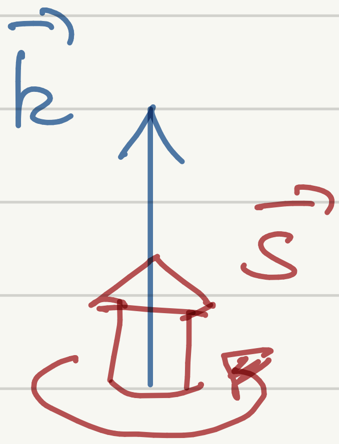
with

$$\lambda = +\frac{\hbar}{2} \qquad u_1 = \begin{pmatrix}1\\0\end{pmatrix}$$

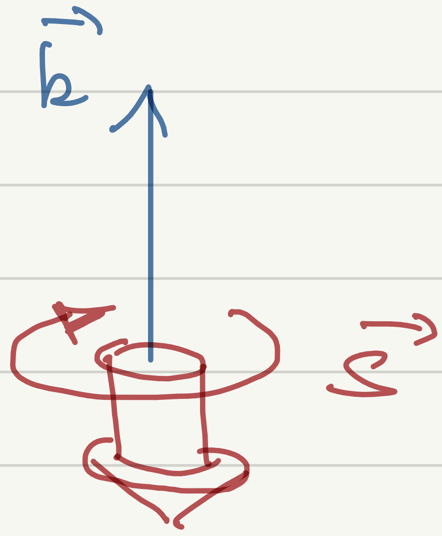
(444)

$$\lambda = -\frac{\hbar}{2} \qquad u_{-1} = \begin{pmatrix}0\\1\end{pmatrix}$$

$\boxed{u_1}$



$\boxed{u_{-1}}$



With this we can fully classify all solutions of the free Dirac equation for $\vec{k} = k\vec{e}_z$

$$\boxed{\begin{aligned} \psi_{\vec{k},\lambda,+\frac{1}{2}} &= N \begin{pmatrix} 1 \\ 0 \\ \dfrac{c\hbar k}{m_0c^2+\lambda E_p}\begin{pmatrix}1\\0\end{pmatrix} \end{pmatrix} e^{i(kz-\lambda E_p/\hbar\, t)} \qquad (445) \\ \psi_{\vec{k},\lambda,-\frac{1}{2}} &= N \begin{pmatrix} 1 \\ 0 \\ -\dfrac{c\hbar k}{m_0c^2+\lambda E_p}\begin{pmatrix}0\\1\end{pmatrix} \end{pmatrix} e^{i(kz-\lambda E_p/\hbar\, t)} \end{aligned}}$$

(C) Dirac field in an external elm. field and non-relativistic limit of DE

principle of minimal coupling as in Klein-Gordon theory

$$\hat{p}^\mu \longrightarrow \hat{p}^\mu - \frac{e}{c} A^\mu$$

i.e.

(446) $$\boxed{i\hbar \frac{\partial}{\partial t} \Psi = \left(c\, \vec{\alpha} \left(\hat{\vec{p}} - \frac{e}{c} \vec{A} \right) + eA_0 + \beta m_0 c^2 \right) \Psi}$$

As in the KG-theory this equation is invariant under gauge-phase transformation or shortly gauge-trafo

(447) $$\boxed{\begin{aligned} A_\mu(x) &\to A'_\mu(x) = A_\mu(x) + \frac{\partial}{\partial x^\mu} \lambda(x) \\ \Psi(x) &\to \Psi'(x) = \Psi(x) \exp\left(-\frac{ie\lambda(x)}{\hbar c} \right) \end{aligned}}$$

It is interesting to consider the non-relativistic limit of (446) with ansatz (similar to K-G-theory)

(448) $$\Psi(\vec{r}, t) = \begin{pmatrix} \varphi(\vec{r}, t) \\ \chi(\vec{r}, t) \end{pmatrix} e^{-i(m_0 c^2/\hbar)t}$$

this yields

$$(449) \quad i\hbar\frac{\partial}{\partial t}\begin{pmatrix}\varphi\\ \chi\end{pmatrix} = \begin{pmatrix} c\vec{\sigma}\cdot\hat{\vec{\pi}}\,\chi \\ c\vec{\sigma}\cdot\hat{\vec{\pi}}\,\varphi\end{pmatrix} + eA_0\begin{pmatrix}\varphi\\ \chi\end{pmatrix} - 2m_0c^2\begin{pmatrix}0\\ \chi\end{pmatrix}$$

where $\hat{\vec{\pi}} \equiv \hat{\vec{p}} - \frac{e}{c}\vec{A}$ and φ, χ are slowly varying on time scale $(m_0c^2/\hbar)^{-1}$ i.e.

$$(450) \quad \left| i\hbar\frac{\partial}{\partial t}\chi\right| \ll \left| m_0c^2\chi\right| \qquad \left|eA_0\chi\right| \ll \left|m_0c^2\varphi\right|$$

$\Rightarrow$ in eq. for χ the term $-2m_0c^2\chi$ is dominant!

$$(451) \quad \chi \simeq \frac{\vec{\sigma}\cdot\hat{\vec{\pi}}}{2m_0c}\varphi \quad \text{i.e.} \quad \boxed{|\chi| \ll |\varphi|}$$

$$\Rightarrow \quad (452) \quad i\hbar\frac{\partial}{\partial t}\varphi = \frac{(\vec{\sigma}\cdot\hat{\vec{\pi}})(\vec{\sigma}\cdot\hat{\vec{\pi}})}{2m_0}\varphi + eA_0\varphi$$

You will show in the problem course that

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

$$= \left(\vec{p} - \frac{e}{c}\vec{A}\right)^2 + i\vec{\sigma}\cdot\left[\left(-i\hbar\vec{\nabla} - \frac{e}{c}\vec{A}\right)\times\left(-i\hbar\vec{\nabla} - \frac{e}{c}\vec{A}\right)\right]$$

only relevant terms

$$(453) \quad = \left(\vec{p} - \frac{e}{c}\vec{A}\right)^2 - \frac{e\hbar}{c}\vec{\sigma}\cdot\underbrace{(\vec{\nabla}\times\vec{A})}_{=\vec{B}}$$

this yields the Pauli equation for a two component spinor $\varphi = \begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix}$

$$\boxed{i\hbar \frac{\partial}{\partial t}\varphi = \left[\frac{1}{2m_0}\left(\vec{p}-\frac{e}{c}\vec{A}\right)^2 - \frac{e}{2m_0 c} 2\vec{S}\cdot\vec{B} + eA_0\right]\varphi \quad (454)}$$

Pauli equation

- $\vec{S} = \frac{\hbar}{2}\vec{\sigma}$ spin
- coupling to magnetic field with g factor 2

The Dirac equation explains the spin and produces the correct gyromagnetic factor!

special case: homogeneous magnetic field

(455) $\vec{A} = \frac{1}{2}(\vec{B}\times\vec{r})$ neglect $\vec{A}^2$ term

$$\left(\vec{p}-\frac{e}{c}\vec{A}\right)^2 = \left(\vec{p}-\frac{e}{2c}(\vec{B}\times\vec{r})\right)^2 \simeq \vec{p}^{\,2} - \frac{e}{c}(\vec{B}\times\vec{r})\cdot\vec{p}$$

(456) $$= \vec{p}^{\,2} - \frac{e}{c}\vec{B}\,\vec{L} \qquad \vec{L} = \vec{r}\times\vec{p}$$

$$\boxed{i\hbar\frac{\partial}{\partial t}\varphi = \left(\frac{\vec{p}^{\,2}}{2m_0} - \frac{e}{2m_0 c}(\vec{L}+2\vec{S})\cdot\vec{B} + eA_0\right)\varphi}$$