Dirac relativistic electron theory

Masatsugu Sei Suzuki
Department of Physics, SUNY at Binghamton
(Date: January 10, 2014)

I taught the advanced quantum mechanics for the graduate students about 10 years ago. Recently I have an opportunity to read my lecture notes (hand written) on the Dirac theory. I realized that my lecture notes are still useful to the students who study the relativistic quantum mechanics. So I revised my old lecture notes. This time I use the Mathematica for the calculation of the commutation relations of Dirac matrices, eigenvalue problems, the calculation of exponent of the matrices, series expansion for the relativistic hydrogen atom, and so on. The complicated mathematical calculations can be replaced by simple Mathematica calculations.

In particle physics, the **Dirac equation** is a relativistic wave equation derived by British physicist Paul Dirac in 1928 and later seen to be an elaboration of the work of Wolfgang Pauli. In its free form, or including electromagnetic interactions, it describes all spin-½ particles, such as electrons and quarks, and is consistent with both the principles of quantum mechanics and the theory of special relativity, and was the first theory to account fully for special relativity in the context of quantum mechanics.

It accounted for the fine details of the hydrogen spectrum in a completely rigorous way. The equation also implied the existence of a new form of matter, *antimatter*, hitherto unsuspected and unobserved, and actually predated its experimental discovery. It also provided a *theoretical* justification for the introduction of several-component wave functions in Pauli's phenomenological theory of spin; the wave functions in the Dirac theory are vectors of four complex numbers (known as bispinors), two of which resemble the Pauli wavefunction in the non-relativistic limit, in contrast to the Schrödinger equation which described wave functions of only one complex value. Moreover, in the limit of zero mass, the Dirac equation reduces to the Weyl equation.

http://en.wikipedia.org/wiki/Dirac_equation

http://en.wikipedia.org/wiki/Paul_Dirac

We discuss the relativistic theory of electron which was derived by Dirac. Here we use the notations

$$x_1 = x, \qquad x_2 = y, \qquad x_3 = z, \qquad x_4 = ict \qquad (x_0 = ct)$$

$$p_1 = \frac{\hbar}{i}\frac{\partial}{\partial x_1} = \frac{\hbar}{i}\frac{\partial}{\partial x}, \qquad p_2 = \frac{\hbar}{i}\frac{\partial}{\partial x_2} = \frac{\hbar}{i}\frac{\partial}{\partial y}, \qquad p_3 = \frac{\hbar}{i}\frac{\partial}{\partial x_3} = \frac{\hbar}{i}\frac{\partial}{\partial z}$$

$$p_4 = \frac{\hbar}{i}\frac{\partial}{\partial x_4} = \frac{\hbar}{i}\frac{\partial}{\partial (ict)} = -\frac{\hbar}{c}\frac{\partial}{\partial t} = \frac{i}{c}E$$

$$x_k = (x, y, z), \qquad p_k = (p_x, p_y, p_z)$$

$$x_\mu = (x_1, x_2, x_3, x_4), \qquad p_\mu = (p_1, p_2, p_3, p_4)$$

We also use the abbreviation for the summations,

$$x_k p_k = \sum_{k=1}^{3} x_k p_k, \qquad x_\mu p_\mu = \sum_{\mu=1}^{4} x_\mu p_\mu$$

1. One particle theory

We consider the simplest case, one particle with no forces. The energy of the particle is given by

$$E = \frac{1}{2m}\boldsymbol{p}^2 .$$

Using the relation

$$E = i\hbar\frac{\partial}{\partial t}, \qquad \boldsymbol{p} \to \frac{\hbar}{i}\nabla ,$$

we get the Schrodinger equation for the wave function ψ,

$$i\hbar\frac{\partial}{\partial t}\psi = -\frac{\hbar^2}{2m}\nabla^2\psi .$$

In order to give a physical meaning to ψ, we state that

$$\rho = \psi^*\psi .$$

is the probability of finding the particle at the point (x, y, z) at time t. The Probability current density is

$$\boldsymbol{J} = \mathrm{Re}(\psi^* \frac{p}{m}\psi) = \mathrm{Re}(\psi^* \frac{\hbar}{mi}\nabla\psi) = \frac{\hbar}{2mi}(\psi^*\nabla\psi - \psi\nabla\psi^* .$$

The probability is conserved because

$$\frac{\partial\rho}{\partial t} + \nabla\cdot\boldsymbol{J} = 0,$$

What happens to the particle relativistically. The energy of particle is given by

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

which leads to the Klein-Gordon equation,

$$\frac{1}{c^2}\frac{\partial^2}{\partial t^2}\psi = \nabla^2\psi - \frac{m^2c^2}{\hbar^2}\psi$$

In order to give a physical meaning to ψ, we must have a continuity equation. This condition $\frac{\partial\rho}{\partial t} + \nabla\cdot\boldsymbol{J} = 0$ can be satisfied only if we take $\boldsymbol{J}$ as before and

$$\rho = \frac{i\hbar}{2mc^2}(\psi^* \frac{\partial \psi}{\partial t} - \psi \frac{\partial \psi^*}{\partial t})$$

Note that

$$\begin{aligned}
\frac{\partial \rho}{\partial t} &= \frac{i\hbar}{2m}(\psi^* \frac{1}{c^2}\frac{\partial^2 \psi}{\partial^2 t} - \psi \frac{1}{c^2}\frac{\partial^2 \psi^*}{\partial t^2}) \\
&= \frac{i\hbar}{2m}[\psi^*(\nabla^2 \psi - \frac{m^2c^2}{\hbar^2}\psi) - \psi(\nabla^2 \psi^* - \frac{m^2c^2}{\hbar^2}\psi^*)] \\
&= -\frac{\hbar}{2mi}(\psi^* \nabla^2 \psi - \psi \nabla^2 \psi) \\
&= -\nabla \cdot \boldsymbol{J}
\end{aligned}$$

The probability density thus defined is not always positive. We have negative probability.

2 Hamiltonian

The time dependent Schrödinger equation for the particle is given by

$$i\hbar \frac{\partial}{\partial t}\psi = -\frac{\hbar^2}{2m}\nabla^2 \psi$$

We find that the time t and the space position (x, y, z) are treated very non symmetrically. We need to search for relativistic equation for the particle of first order in t, x, y, and z, where the equation should be symmetrical in space and time coordinates. Thus H is required to be linear in the momentum operator.

$$i\hbar \frac{\partial}{\partial t}\psi = H\psi$$

The form of H is introduced by Dirac as

$$H = c\boldsymbol{\alpha} \cdot \boldsymbol{p} + \beta mc^2$$

By squaring H, we should get the relation from the relativity (the Einstein relation),

$$\begin{aligned}
H^2 &= (c\boldsymbol{\alpha} \cdot \boldsymbol{p} + \beta mc^2)^2 = c^2[p_i p_j \frac{1}{2}\{\alpha_i, \alpha_j\} + mcp_i\{\alpha_i, \beta\} + \beta^2 m^2 c^2] \\
&= m^2c^4 + c^2\boldsymbol{p}^2 = E^2
\end{aligned}$$

which leads to the relations

$$\{\alpha_i,\alpha_j\} = 2\delta_{ij} I\,, \qquad \{\alpha_i,\beta\} = 0\,, \qquad \beta^2 = I$$

where the curly bracket denotes an anti-commutator,

$$\{\alpha_i,\alpha_j\} = \alpha_i\alpha_j + \alpha_j\alpha_i$$

Here we do not show how to derive the form of matrices α and β (4 x 4). The matrices are Hermitian matrices (4x4). Thus the Hamiltonian is also Hermitian.

3. The matrices α and β

The matrices $\boldsymbol{\alpha}$ and β can be expressed in terms of the Pauli spin matrices,

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

$$I_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

Using the Kronecker product, the matrices α_x, α_y, α_z, and β are given by

$$\alpha_1 = \sigma_1 \otimes \sigma_1 = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & \sigma_1 \\ \sigma_1 & 0 \end{pmatrix}$$

$$\alpha_2 = \sigma_2 \otimes \sigma_2 = \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & \sigma_2 \\ \sigma_2 & 0 \end{pmatrix}$$

$$\alpha_3 = \sigma_3 \otimes \sigma_3 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & \sigma_3 \\ \sigma_3 & 0 \end{pmatrix}$$

$$\beta = \sigma_z \otimes I_2 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} = \begin{pmatrix} I_2 & 0 \\ 0 & -I_2 \end{pmatrix}$$

$$\gamma_1 = -i\beta\alpha_1 = \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & -i & 0 \\ 0 & i & 0 & 0 \\ i & 0 & 0 & 0 \end{pmatrix},$$

$$\gamma_2 = -i\beta\alpha_2 = \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}$$

$$\gamma_3 = -i\beta\alpha_3 = \begin{pmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & i \\ i & 0 & 0 & 0 \\ 0 & -i & 0 & 0 \end{pmatrix}$$

$$\beta = \gamma_4 = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}$$

$$\alpha_k = i\gamma_4\gamma_k = \begin{pmatrix} 0 & \sigma_k \\ \sigma_k & 0 \end{pmatrix}$$

$$\gamma_4\gamma_k = -\gamma_k\gamma_4$$

The Hamiltonian H is described by

$$H = \begin{pmatrix} mc^2 & 0 & cp_z & c(p_x - ip_y) \\ 0 & mc^2 & c(p_x + ip_y) & -cp_z \\ cp_z & c(p_x - ip_y) & -mc^2 & 0 \\ c(p_x + ip_y) & -cp_z & 0 & -mc^2 \end{pmatrix}$$

H^2 can be evaluated as

$$H^2 = E^2 \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} = E^2 I_4$$

where

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

((**Mathematica**))

```
Clear["Global`*"]; σx = (0 1
                         1 0); σy = (0 -ⅈ
                                     ⅈ  0);
σz = (1  0
      0 -1); I2 = IdentityMatrix[2];
```

```
αx = KroneckerProduct[σx, σx];
αx // MatrixForm
```

$$\begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}$$

```
αy = KroneckerProduct[σx, σy];
αy // MatrixForm
```

$$\begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \end{pmatrix}$$

```
αz = KroneckerProduct[σx, σz];
αz // MatrixForm
```

$$\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}$$

```
β = KroneckerProduct[σz, I2]; β // MatrixForm
```

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

```
γx = -ⅈ β.αx // Simplify; γx // MatrixForm
```

$$\begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & -i & 0 \\ 0 & i & 0 & 0 \\ i & 0 & 0 & 0 \end{pmatrix}$$

```
γy = -ⅈ β.αy // Simplify; γy // MatrixForm
```

$$\begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}$$

```
γz = -ⅈ β.αz // Simplify; γz // MatrixForm
```

$$\begin{pmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & i \\ i & 0 & 0 & 0 \\ 0 & -i & 0 & 0 \end{pmatrix}$$

```
f1 = c px αx + c py αy + c pz αz + β m^2 c^2
```

$$\{\{c^2 m^2, 0, c\,pz, c\,px - i\,c\,py\},$$
$$\{0, c^2 m^2, c\,px + i\,c\,py, -c\,pz\},$$
$$\{c\,pz, c\,px - i\,c\,py, -c^2 m^2, 0\},$$
$$\{c\,px + i\,c\,py, -c\,pz, 0, -c^2 m^2\}\}$$

```
g1 = f1.f1 // FullSimplify
```

$$\{\{c^2 (c^2 m^4 + px^2 + py^2 + pz^2), 0, 0, 0\},$$
$$\{0, c^2 (c^2 m^4 + px^2 + py^2 + pz^2), 0, 0\},$$
$$\{0, 0, c^2 (c^2 m^4 + px^2 + py^2 + pz^2), 0\},$$
$$\{0, 0, 0, c^2 (c^2 m^4 + px^2 + py^2 + pz^2)\}\}$$

4. Dirac equation

We now have the Dirac equation given by

$$i\hbar\frac{\partial}{\partial t}\psi = H\psi$$

with

$$H = c\boldsymbol{\alpha}\cdot\boldsymbol{p} + \beta mc^2$$

Then we get

$$i\hbar\frac{\partial}{\partial(ct)}\psi = (\boldsymbol{\alpha}\cdot\boldsymbol{p} + \beta mc)\psi = (i\gamma_4\boldsymbol{\gamma}\cdot\frac{\hbar}{i}\nabla + \beta mc)\psi$$

or

$$[\gamma_k\cdot\frac{\partial}{\partial x_k} + \gamma_4\frac{\partial}{\partial(ix_0)} + \frac{mc}{\hbar}]\psi = 0,$$

with $x_1=x$, $x_2 = y$, $x_3 = z$, and $x_4 = ict.$, since

$$\boldsymbol{\alpha} = i\gamma_4\boldsymbol{\gamma}, \qquad \gamma_4^{\ 2} = 1, \qquad \beta = \gamma_4$$

Simply we have

$$(\gamma_\mu\frac{\partial}{\partial x_\mu} + \frac{mc}{\hbar})\psi = 0$$

where μ = 1, 2, 3, and 4.

5. Alternative method (Sakurai)

$$\frac{E^2}{c^2} - \boldsymbol{p}^2 = m^2c^2$$

$$(\frac{E^{(op)}}{c} - \boldsymbol{\sigma}\cdot\boldsymbol{p})(\frac{E^{(op)}}{c} + \boldsymbol{\sigma}\cdot\boldsymbol{p}) = m^2c^2$$

where

$$E^{(op)} = i\hbar\frac{\partial}{\partial t} = i\hbar c\frac{\partial}{\partial x_0}$$

with $x_0 = ct$

This enables us to write a second order equation

$$(i\hbar\frac{\partial}{\partial x_0} + i\hbar\boldsymbol{\sigma}\cdot\nabla)(i\hbar\frac{\partial}{\partial x_0} - i\hbar\boldsymbol{\sigma}\cdot\nabla)\phi = m^2c^2\phi$$

for a free electron. ϕ is now a two component wave function

$$\phi^{(R)} = \frac{1}{mc}(i\hbar\frac{\partial}{\partial x_0} - i\hbar\boldsymbol{\sigma}\cdot\nabla)\phi$$

and

$$\phi^{(L)} = \phi$$

$$(i\hbar\frac{\partial}{\partial x_0} + i\hbar\boldsymbol{\sigma}\cdot\nabla)\phi^{(R)} = mc\phi^{(L)}$$

or

$$(-i\hbar\frac{\partial}{\partial x_0} - i\hbar\sigma\cdot\nabla)\phi^{(R)} = -mc\phi^{(L)} \tag{1a}$$

and

$$(-i\hbar\frac{\partial}{\partial x_0} + i\hbar\sigma\cdot\nabla)\phi^{(L)} = -mc\phi^{(R)} \tag{1b}$$

((Dirac equation))

Taking the sum and the difference of Eq.(1).

$$-i\hbar\boldsymbol{\sigma}\cdot\nabla(\phi^{(R)} - \phi^{(L)}) - i\hbar\frac{\partial}{\partial x_0}(\phi^{(R)} + \phi^{(L)}) = -mc(\phi^{(R)} + \phi^{(L)})$$

$$i\hbar\boldsymbol{\sigma}\cdot\nabla(\phi^{(R)} + \phi^{(L)}) + i\hbar\frac{\partial}{\partial x_0}(\phi^{(R)} - \phi^{(L)}) = -mc(\phi^{(R)} - \phi^{(L)})$$

We define

$$\psi_A = \phi^{(R)} + \phi^{(L)}$$

and

$$\psi_B = \phi^{(R)} - \phi^{(L)}$$

Then

$$-i\hbar\boldsymbol{\sigma}\cdot\nabla\psi_B - i\hbar\frac{\partial}{\partial x_0}\psi_A = -mc\psi_A$$

$$i\hbar\boldsymbol{\sigma}\cdot\nabla\psi_A + i\hbar\frac{\partial}{\partial x_0}\psi_B = -mc\psi_B$$

$$\begin{pmatrix} -i\hbar\frac{\partial}{\partial x_0} & -i\hbar\boldsymbol{\sigma}\cdot\nabla \\ i\hbar\boldsymbol{\sigma}\cdot\nabla & i\hbar\frac{\partial}{\partial x_0} \end{pmatrix}\begin{pmatrix}\psi_A \\ \psi_B\end{pmatrix} = -mc\begin{pmatrix}\psi_A \\ \psi_B\end{pmatrix}$$

$\begin{pmatrix}\psi_A \\ \psi_B\end{pmatrix}$ is the 4x1 column matrix.

Here note that

$$\begin{pmatrix} -i\hbar\frac{\partial}{\partial x_0} & -i\hbar\boldsymbol{\sigma}\cdot\nabla \\ i\hbar\boldsymbol{\sigma}\cdot\nabla & i\hbar\frac{\partial}{\partial x_0} \end{pmatrix} = \hbar\frac{\partial}{\partial(ix_0)}\begin{pmatrix} I & 0 \\ 0 & -I\end{pmatrix} + \hbar\begin{pmatrix} 0 & -i\sigma \\ i\sigma & 0\end{pmatrix}\cdot\nabla$$

γ_μ: gamma matrices (or Dirac matrices)

$$\gamma_4 = \begin{pmatrix} I & 0 \\ 0 & -I\end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1\end{pmatrix}$$

and

$$\gamma_1 = \begin{pmatrix} 0 & -i\sigma_1 \\ i\sigma_1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & -i & 0 \\ 0 & i & 0 & 0 \\ i & 0 & 0 & 0 \end{pmatrix}$$

$$\gamma_2 = \begin{pmatrix} 0 & -i\sigma_2 \\ i\sigma_2 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}$$

$$\gamma_3 = \begin{pmatrix} 0 & -i\sigma_3 \\ i\sigma_3 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & i \\ i & 0 & 0 & 0 \\ 0 & -i & 0 & 0 \end{pmatrix}$$

with

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Dirac spinor

$$\psi = \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix} = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix}$$

Using these definitions, we have Dirac equation

$$[\boldsymbol{\gamma} \cdot \nabla + \gamma_4 \frac{\partial}{\partial(ix_0)} + \frac{mc}{\hbar}]\psi = 0$$

with

$$\{\gamma_\mu, \gamma_\nu\} = \gamma_\mu\gamma_\nu + \gamma_\nu\gamma_\mu = 2\delta_{\mu\nu}$$

$$\gamma_\mu{}^+ = \gamma_\mu \qquad \text{(Hermutian)}$$

For example

$$
\begin{aligned}
\{\gamma_1,\gamma_2\} &= \gamma_1\gamma_2+\gamma_2\gamma_1 \\
&= \begin{pmatrix} 0 & -i\sigma_1 \\ i\sigma_1 & 0 \end{pmatrix}\begin{pmatrix} 0 & -i\sigma_2 \\ i\sigma_2 & 0 \end{pmatrix} + \begin{pmatrix} 0 & -i\sigma_2 \\ i\sigma_2 & 0 \end{pmatrix}\begin{pmatrix} 0 & -i\sigma_1 \\ i\sigma_1 & 0 \end{pmatrix} \\
&= \begin{pmatrix} [\sigma_1,\sigma_2]_+ & 0 \\ 0 & [\sigma_1,\sigma_2]_+ \end{pmatrix} \\
&= 0
\end{aligned}
$$

where

$$[\sigma_1,\sigma_2]_+ = \sigma_1\sigma_2+\sigma_2\sigma_1 = 0$$

6. Lorentz invariance of the Dirac equation

6.1. Lorentz transformation

$$a = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \gamma & -i\beta\gamma \\ 0 & 0 & i\beta\gamma & \gamma \end{pmatrix} \qquad a^T = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \gamma & i\beta\gamma \\ 0 & 0 & -i\beta\gamma & \gamma \end{pmatrix}$$

$$\det(a) = 1$$

$$a^{-1} = a^T$$

$$\left(a^{-1}\right)_{\mu\nu} = \left(a^T\right)_{\mu\nu} = a_{\nu\mu}$$

$$x_\mu' = a_{\mu\nu}x_\nu, \qquad a_{\mu\nu}x_\mu' = a_{\mu\nu}a_{\mu\lambda}x_\lambda = \delta_{\nu\lambda}x_\lambda = x_\nu$$

$$x_\mu' x_\mu' = a_{\mu\nu}a_{\mu\rho}x_\nu x_\rho = \delta_{\nu\rho}x_\nu x_\rho = x_\mu x_\mu$$

$$a_{\mu\nu}a_{\mu\rho} = \delta_{\nu\rho}$$

$$a(\beta_1)a(\beta_2) = a(\beta_{12})$$

with

$$\beta_{12} = \frac{\beta_1 + \beta_2}{1 + \beta_1 \beta_2}.$$

6.2. Relativistic co-variance

$$\gamma_\mu \frac{\partial}{\partial x_\mu '} \psi'(x') + \frac{mc}{\hbar} \psi'(x') = 0$$

where

γ_μ is not primed.

$$x_\mu ' = a_{\mu\nu} x_\nu$$
$$x_\nu = a_{\mu\nu} x_\mu '$$

$$\psi' = S\psi .$$

where S is a 4 x 4 matrix. We note that

$$\frac{\partial}{\partial x_\mu '} = \frac{\partial x_\nu}{\partial x_\mu '} \frac{\partial}{\partial x_\nu} = a_{\mu\nu} \frac{\partial}{\partial x_\nu}$$

Thus we get

$$\gamma_\mu a_{\mu\nu} \frac{\partial}{\partial x_\nu} S\psi(x) + \frac{mc}{\hbar} S\psi(x) = 0$$

Multiplying S^{-1} from the left, we have

$$S^{-1} \gamma_\mu a_{\mu\nu} \frac{\partial}{\partial x_\nu} S\psi(x) + \frac{mc}{\hbar} \psi(x) = 0$$

or

$$S^{-1} \gamma_\mu S a_{\mu\nu} \frac{\partial}{\partial x_\nu} \psi(x) + \frac{mc}{\hbar} \psi(x) = 0 .$$

If

$$S^{-1} \gamma_\mu S a_{\mu\nu} = \gamma_\nu$$

or

$$S^{-1}\gamma_\lambda S a_{\lambda\nu} a_{\mu\nu} = a_{\mu\nu}\gamma_\nu$$

or

$$S^{-1}\gamma_\mu S = a_{\mu\nu}\gamma_\nu\,,$$

the problem of demonstrating the relativistic covariance of the Dirac equation is now reduced to that of finding the form of *S*.

$$\overline{\psi} = \psi^+\gamma_4 \qquad\qquad \overline{\psi}\gamma_4 = \psi^+\gamma_4{}^2 = \psi^+$$

$$(\frac{\partial}{\partial x_\mu}\psi^+)\gamma_\mu + \frac{mc}{\hbar}\psi^+ = 0\,, \qquad (\frac{\partial}{\partial x_\mu}\overline{\psi}\gamma_4)\gamma_\mu + \frac{mc}{\hbar}\overline{\psi}\gamma_4 = 0$$

or

$$-(\frac{\partial}{\partial x_\mu}\overline{\psi})\gamma_\mu + \frac{mc}{\hbar}\overline{\psi} = 0$$

6.3 Relativistic co-variance

$$-(\frac{\partial}{\partial x_\mu{}'}\overline{\psi}')\gamma_\mu + \frac{mc}{\hbar}\overline{\psi}' = 0\,.$$

From this we get

$$-a_{\mu\nu}\frac{\partial}{\partial x_\nu}\overline{\psi}'\gamma_\mu + \frac{mc}{\hbar}\overline{\psi}' = 0$$

We assume that

$$\overline{\psi}' = \overline{\psi}T^{-1}$$

$$-a_{\mu\nu}\frac{\partial}{\partial x_\nu}\overline{\psi}T^{-1}\gamma_\mu + \frac{mc}{\hbar}\overline{\psi}T^{-1} = 0$$

Multiplying *T* from the left

$$-a_{\mu\nu}\frac{\partial}{\partial x_\nu}\overline{\psi}T^{-1}\gamma_\mu T + \frac{mc}{\hbar}\overline{\psi} = 0$$

$$\gamma_\nu = a_{\mu\nu} T^{-1} \gamma_\mu T = T^{-1} \gamma_\mu T a_{\mu\nu}$$

or

$$T^{-1} \gamma_\mu T = a_{\mu\nu} \gamma_\nu$$

Here we can choose $T = S$. Then we have

$$\overline{\psi} = \psi^+ \gamma_4 , \qquad \overline{\psi}\gamma_4 = \psi^+$$

$$\psi' = S\psi , \qquad \overline{\psi}' = \overline{\psi} S^{-1}$$

since

$$\overline{\psi}' = \psi'^+ \gamma_4 = \overline{\psi}\gamma_4 S^+ \gamma_4 = \overline{\psi} S^{-1}$$

or

$$\gamma_4 S^+ \gamma_4 = S^{-1}$$

or

$$S^+ \gamma_4 = \gamma_4 S^{-1}$$

In summary we have the following relations,

$$S^{-1} \gamma_\mu S = a_{\mu\nu} \gamma_\nu$$

$$S^+ \gamma_4 = \gamma_4 S^{-1}$$

$$\psi' = S\psi$$

$$\overline{\psi}' = \overline{\psi} S^{-1}$$

6.4 Infinitesimal Lorentz transformation

$$a_{\mu\nu} = \delta_{\mu\nu} + \varepsilon_{\mu\nu}$$

with the addition

$$\varepsilon_{\mu\nu} = -\varepsilon_{\nu\mu}$$

since

$$a_{\mu\lambda}a_{\nu\lambda} = \delta_{\mu\nu}$$

$\varepsilon_{\mu\nu}$ is pure-imaginary when one of μ, ν is equal to 4.

((**Note**))

$$a_{\mu\lambda}a_{\nu\lambda} = (\delta_{\mu\lambda} + \varepsilon_{\mu\lambda})(\delta_{\nu\lambda} + \varepsilon_{\nu\lambda}) = \delta_{\mu\nu}$$

or

$$\delta_{\mu\lambda}\delta_{\nu\lambda} + \delta_{\mu\lambda}\varepsilon_{\nu\lambda} + \varepsilon_{\mu\lambda}\delta_{\nu\lambda} + \varepsilon_{\mu\lambda}\varepsilon_{\nu\lambda} = \delta_{\mu\nu}$$

Neglecting $\varepsilon_{\mu\lambda}\varepsilon_{\nu\lambda}$, we get

$$\delta_{\mu\lambda}\delta_{\nu\lambda} + \delta_{\mu\lambda}\varepsilon_{\nu\lambda} + \varepsilon_{\mu\lambda}\delta_{\nu\lambda} = \delta_{\mu\nu}$$

or

$$\delta_{\mu\nu} + \varepsilon_{\nu\mu} + \varepsilon_{\mu\nu} = \delta_{\mu\nu}$$

or

$$\varepsilon_{\nu\mu} = -\varepsilon_{\mu\nu}$$

6.5 The expression of *S*

We now consider the relation

$$S^{-1}\gamma_\mu S = a_{\mu\nu}\gamma_\nu$$

We assume that

$$S = 1 + T + O(T^2)$$

Then we get

$$(1 - T)\gamma_\mu(1 + T) = (\delta_{\mu\nu} + \varepsilon_{\mu\nu})\gamma_\nu$$

or

$$(\gamma_\mu - T\gamma_\mu)(1+T) = \gamma_\mu + \varepsilon_{\mu\nu}\gamma_\nu$$

or

$$\gamma_\mu + [\gamma_\mu, T] = \gamma_\mu + \varepsilon_{\mu\nu}\gamma_\nu$$

or

$$[\gamma_\mu, T] = \varepsilon_{\mu\nu}\gamma_\nu$$

The solution of this commutation relation is seen to be

$$T = \frac{1}{4}\varepsilon_{\mu\nu}\gamma_\mu\gamma_\nu$$

Then we have

$$\begin{aligned} S &= 1 + \frac{1}{4}\varepsilon_{\mu\nu}\gamma_\mu\gamma_\nu \\ &= 1 + \frac{1}{8}\varepsilon_{\mu\nu}[\gamma_\mu, \gamma_\nu] \\ &= 1 + \frac{i}{4}\varepsilon_{\mu\nu}\sigma_{\mu\nu} \end{aligned}$$

where

$$\sigma_{\mu\nu} = \frac{1}{2i}[\gamma_\mu, \gamma_\nu]$$

((**Note-1**))
Noting that

$$\{\gamma_\mu, \gamma_\nu\} = 2\delta_{\mu\nu}$$

we get

$$
\begin{aligned}
[\gamma_\mu, T] &= \frac{1}{4}[\gamma_\mu, \varepsilon_{\nu\lambda}\gamma_\nu\gamma_\lambda] \\
&= \frac{1}{4}\varepsilon_{\nu\lambda}[\gamma_\mu, \gamma_\nu\gamma_\lambda] \\
&= \frac{1}{4}\varepsilon_{\nu\lambda}(\gamma_\mu\gamma_\nu\gamma_\lambda - \gamma_\nu\gamma_\lambda\gamma_\mu) \\
&= \frac{1}{4}\varepsilon_{\nu\lambda}[(-\gamma_\nu\gamma_\mu + 2\delta_{\mu\nu})\gamma_\lambda - \gamma_\nu(-\gamma_\mu\gamma_\lambda + 2\delta_{\mu\lambda})] \\
&= \frac{1}{2}(\varepsilon_{\nu\lambda}\delta_{\mu\nu}\gamma_\lambda - \varepsilon_{\nu\lambda}\gamma_\nu\delta_{\mu\lambda}) \\
&= \frac{1}{2}(\varepsilon_{\mu\nu}\gamma_\nu - \varepsilon_{\nu\mu}\gamma_\nu) = \varepsilon_{\mu\nu}\gamma_\nu
\end{aligned}
$$

((**Note-2**))

$$
\begin{aligned}
\varepsilon_{\mu\nu}\gamma_\mu\gamma_\nu &= \frac{1}{2}(\varepsilon_{\mu\nu}\gamma_\mu\gamma_\nu + \varepsilon_{\nu\mu}\gamma_\nu\gamma_\mu) \\
&= \frac{1}{2}\varepsilon_{\mu\nu}(\gamma_\mu\gamma_\nu - \gamma_\nu\gamma_\mu) \\
&= \frac{1}{2}\varepsilon_{\mu\nu}[\gamma_\mu, \gamma_\nu]
\end{aligned}
$$

6.6 The relation $S^+\gamma_4 = \gamma_4 S^{-1}$

We show that *S* satisfies the relation $S^+\gamma_4 = \gamma_4 S^{-1}$.

$$S = 1 + \frac{1}{4}\varepsilon_{\mu\nu}\gamma_\mu\gamma_\nu$$

$$S^+ = 1 + \frac{1}{4}\varepsilon_{\mu\nu}{}^*\gamma_\nu{}^+\gamma_\mu{}^+ = 1 + \frac{1}{4}\varepsilon_{\mu\nu}{}^*\gamma_\nu\gamma_\mu$$

Then we get

$$S^+\gamma_4 = (1 + \frac{1}{4}\varepsilon_{\mu\nu}{}^*\gamma_\nu\gamma_\mu)\gamma_4 = \gamma_4 + \frac{1}{4}\varepsilon_{\mu\nu}{}^*\gamma_\nu\gamma_\mu\gamma_4$$

$$\gamma_4 S^{-1} = \gamma_4(1 - \frac{1}{4}\varepsilon_{\mu\nu}\gamma_\mu\gamma_\nu) = \gamma_4 - \frac{1}{4}\varepsilon_{\mu\nu}\gamma_4\gamma_\mu\gamma_\nu$$

So we need to show that

$$\varepsilon_{\mu\nu}{}^*\gamma_\nu\gamma_\mu\gamma_4 = -\varepsilon_{\mu\nu}\gamma_4\gamma_\mu\gamma_\nu$$

For $\mu = i$, $\nu = k$ (i, k = 1, 2, 3),

$$\begin{aligned}\varepsilon_{ik}{}^{*}\gamma_k\gamma_i\gamma_4 + \varepsilon_{ik}\gamma_4\gamma_i\gamma_k &= \varepsilon_{ik}(\gamma_k\gamma_i + \gamma_i\gamma_k)\gamma_4 \\ &= \varepsilon_{ik}2\delta_{ik}\gamma_4 \\ &= 0\end{aligned}$$

For $\mu = i$, $\nu = 4$ (i = 1, 2, 3),

$$\begin{aligned}\varepsilon_{i4}{}^{*}\gamma_4\gamma_i\gamma_4 + \varepsilon_{i4}\gamma_4\gamma_i\gamma_4 &= \varepsilon_{i4}\gamma_i\gamma_4{}^{2} - \varepsilon_{i4}\gamma_i\gamma_4{}^{2} \\ &= 0\end{aligned}$$

6.7 Rotation matrices

Infinitesimal rotation

$$a = \begin{pmatrix} \cos\delta\omega & \sin\delta\omega & 0 & 0 \\ -\sin\delta\omega & \cos\delta\omega & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 1 & \delta\omega & 0 & 0 \\ -\delta\omega & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} = 1 + \begin{pmatrix} 0 & \delta\omega & 0 & 0 \\ -\delta\omega & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

$$\varepsilon_{12} = \delta\omega, \qquad \varepsilon_{21} = \delta\omega$$

$$S_{rot} = 1 + \frac{1}{4}\varepsilon_{\mu\nu}\gamma_\mu\gamma_\nu = 1 + \frac{1}{4}(\varepsilon_{12}\gamma_1\gamma_2 + \varepsilon_{21}\gamma_2\gamma_1) = 1 + \frac{1}{4}\delta\omega_{12}[\gamma_1, \gamma_2] = 1 + \frac{1}{2}i\delta\omega\sigma_{12}$$

where

$$\sigma_{12} = \Sigma_3 = -i\gamma_1\gamma_2$$

Finite rotation

$$\begin{aligned}S_{rot}(\omega) &= \lim_{N\to\infty}[S_{rot}(\delta\omega)]^N \\ &= \lim_{N\to\infty}(1 + \frac{1}{2}i\frac{\omega}{N}\Sigma_3)^N \\ &= \exp(i\frac{1}{2}\omega\Sigma_3) \\ &= 1\cos\frac{\omega}{2} + i\sin\frac{\omega}{2}\Sigma_3\end{aligned}$$

where

$$\omega = N\delta\omega$$

Note that

$$S_{rot}(\omega) = \begin{pmatrix} e^{\frac{i\omega}{2}} & 0 & 0 & 0 \\ 0 & e^{-\frac{i\omega}{2}} & 0 & 0 \\ 0 & 0 & e^{\frac{i\omega}{2}} & 0 \\ 0 & 0 & 0 & e^{-\frac{i\omega}{2}} \end{pmatrix}$$

$$S_{rot}(\omega)^{-1}\gamma_1 S_{rot}(\omega) = \gamma_1 \cos\omega + \gamma_2 \sin\omega$$

$$S_{rot}(\omega)^{-1}\gamma_2 S_{rot}(\omega) = -\gamma_1 \sin\omega + \gamma_2 \cos\omega$$

((Mathematica))

```
Clear["Global`*"];
exp_* := exp /. {Complex[re_, im_] :→ Complex[re, -im]};
σx = (0 1
      1 0); σy = (0 -ⅈ
                  ⅈ  0); σz = (1  0
                              0 -1); I2 = IdentityMatrix[2];
I4 = IdentityMatrix[4];

αx = KroneckerProduct[σx, σx]; αy = KroneckerProduct[σx, σy];
αz = KroneckerProduct[σx, σz];
β = KroneckerProduct[σz, I2];

γ1 = -ⅈ β.αx // Simplify; γ2 = -ⅈ β.αy // Simplify;
γ3 = -ⅈ β.αz // Simplify; γ4 = β; Σ1 = -ⅈ γ2.γ3; Σ2 = -ⅈ γ2.γ3;
Σ3 = -ⅈ γ1.γ2; S1 = MatrixExp[ⅈ/2 ω Σ3];

S1 // MatrixForm
```

$$\begin{pmatrix} e^{\frac{i\omega}{2}} & 0 & 0 & 0 \\ 0 & e^{-\frac{i\omega}{2}} & 0 & 0 \\ 0 & 0 & e^{\frac{i\omega}{2}} & 0 \\ 0 & 0 & 0 & e^{-\frac{i\omega}{2}} \end{pmatrix}$$

```
MatrixExp[ⅈ/2 ω Σ3] - (Cos[ω/2] I4 + I Sin[ω/2] Σ3) // Simplify
```

```
{{0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}}
```

```
Inverse[S1].γ1.S1 - (γ1 Cos[ω] + γ2 Sin[ω]) // Simplify
```

```
{{0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}}
```

```
Inverse[S1].γ2.S1 - (-γ1 Sin[ω] + γ2 Cos[ω]) // Simplify
```

```
{{0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}}
```

6.8 Lorentz transformation

The Lorentz transformation is expressed by

$$a = \begin{pmatrix} \cosh\chi & 0 & 0 & i\sinh\chi \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -i\sinh\chi & 0 & 0 & \cosh\chi \end{pmatrix}$$

where

$$\beta = \tanh\chi, \qquad \cosh\chi = \gamma, \qquad \sinh\chi = \beta\gamma$$

The pure Lorentz transformation is nothing more than a rotation in the 1-4 plane by imaginary angle;

$$S_{rot}(\omega) = 1\cos\frac{\omega}{2} + i\sin\frac{\omega}{2}(-i\gamma_1\gamma_2) = 1\cos\frac{\omega}{2} + \sin\frac{\omega}{2}\gamma_1\gamma_2$$

$$\omega \to i\chi\,, \qquad \gamma_2 \to \gamma_4$$

Then we have

$$S_{Lor} = 1\cosh\frac{\chi}{2} + i\gamma_1\gamma_4\sinh\frac{\chi}{2} = \begin{pmatrix} \cosh\frac{\chi}{2} & 0 & 0 & -\sinh\frac{\chi}{2} \\ 0 & \cosh\frac{\chi}{2} & -\sinh\frac{\chi}{2} & 0 \\ 0 & -\sinh\frac{\chi}{2} & \cosh\frac{\chi}{2} & 0 \\ -\sinh\frac{\chi}{2} & 0 & 0 & \cosh\frac{\chi}{2} \end{pmatrix}$$

where

$$\cos\frac{\omega}{2} = \cosh\frac{\chi}{2}, \qquad \sin\frac{\omega}{2} = i\sinh\frac{\chi}{2}$$

The Hermitian conjugate of S_{Lor} is obtained by

$$\begin{aligned} S_{Lor}{}^{+} &= 1\cosh\frac{\chi}{2} - i\gamma_4{}^{+}\gamma_1{}^{+}\sinh\frac{\chi}{2} \\ &= 1\cosh\frac{\chi}{2} - i\gamma_4\gamma_1\sinh\frac{\chi}{2} \\ &= 1\cosh\frac{\chi}{2} + i\gamma_1\gamma_4\sinh\frac{\chi}{2} \\ &= S_{Lor} \end{aligned}$$

and

$$S_{Lor}{}^{-1} = \cosh\frac{\chi}{2} - i\gamma_1\gamma_4\sinh\frac{\chi}{2} = \begin{pmatrix} \cosh\frac{\chi}{2} & 0 & 0 & \sinh\frac{\chi}{2} \\ 0 & \cosh\frac{\chi}{2} & \sinh\frac{\chi}{2} & 0 \\ 0 & \sinh\frac{\chi}{2} & \cosh\frac{\chi}{2} & 0 \\ \sinh\frac{\chi}{2} & 0 & 0 & \cosh\frac{\chi}{2} \end{pmatrix}$$

Thus S_{Lor} is not unitary. It is important to note that for both pure rotation and pure Lorentz transformation, we have

$$S^{-1} = \gamma_4 S^{+}\gamma_4, \qquad S^{+} = \gamma_4 S - 1^{+}\gamma_4$$

((**Note**))

$$\psi'^{+}\psi' = \psi^{+}S_{Lor}{}^{+}S_{Lor}\psi =$$

((**Mathematica**))

```
Clear["Global`*"];
exp_* := exp /. {Complex[re_, im_] :> Complex[re, -im]};
σx = {{0, 1}, {1, 0}}; σy = {{0, -ⅈ}, {ⅈ, 0}}; σz = {{1, 0}, {0, -1}}; I2 = IdentityMatrix[2];
I4 = IdentityMatrix[4];

αx = KroneckerProduct[σx, σx]; αy = KroneckerProduct[σx, σy];
αz = KroneckerProduct[σx, σz];
β = KroneckerProduct[σz, I2];

γ1 = -ⅈ β.αx // Simplify; γ2 = -ⅈ β.αy // Simplify;
γ3 = -ⅈ β.αz // Simplify; γ4 = β; Σ1 = -ⅈ γ2.γ3;
S1 = I4 Cosh[χ/2] + ⅈ γ1 .γ4 Sinh[χ/2];

S1 // MatrixForm
```

$$\begin{pmatrix} \text{Cosh}\left[\frac{\chi}{2}\right] & 0 & 0 & -\text{Sinh}\left[\frac{\chi}{2}\right] \\ 0 & \text{Cosh}\left[\frac{\chi}{2}\right] & -\text{Sinh}\left[\frac{\chi}{2}\right] & 0 \\ 0 & -\text{Sinh}\left[\frac{\chi}{2}\right] & \text{Cosh}\left[\frac{\chi}{2}\right] & 0 \\ -\text{Sinh}\left[\frac{\chi}{2}\right] & 0 & 0 & \text{Cosh}\left[\frac{\chi}{2}\right] \end{pmatrix}$$

```
S1H = Transpose[S1*]; S1H - S1 // Simplify
```

```
{{0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}}
```

```
Inverse[S1] // Simplify; % // MatrixForm
```

$$\begin{pmatrix} \text{Cosh}\left[\frac{\chi}{2}\right] & 0 & 0 & \text{Sinh}\left[\frac{\chi}{2}\right] \\ 0 & \text{Cosh}\left[\frac{\chi}{2}\right] & \text{Sinh}\left[\frac{\chi}{2}\right] & 0 \\ 0 & \text{Sinh}\left[\frac{\chi}{2}\right] & \text{Cosh}\left[\frac{\chi}{2}\right] & 0 \\ \text{Sinh}\left[\frac{\chi}{2}\right] & 0 & 0 & \text{Cosh}\left[\frac{\chi}{2}\right] \end{pmatrix}$$

```
Inverse[S1] - γ4 .S1H.γ4 // Simplify
```

```
{{0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}}
```

$$\texttt{Inverse[S1] - I4 Cosh}\left[\frac{\chi}{2}\right] + i\,\gamma 1.\gamma 4\,\texttt{Sinh}\left[\frac{\chi}{2}\right] \texttt{ // Simplify}$$

```
{{0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}}
```

```
S1H - γ4 .Inverse[S1].γ4 // Simplify
```

```
{{0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}}
```

```
Eigensystem[S1] // FullSimplify
```

$$\left\{\left\{e^{-\chi/2}, e^{-\chi/2}, e^{\chi/2}, e^{\chi/2}\right\}, \{\{1, 0, 0, 1\}, \{0, 1, 1, 0\}, \{-1, 0, 0, 1\}, \{0, -1, 1, 0\}\}\right\}$$

7. Space Inversion (parity operator)

7.1 Definition

When $\boldsymbol{r}' = -\boldsymbol{r}$ and $t' = t$,

$$a = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

det(a) = -1: improper Lorentz transformation.

Under the parity operation,

$$\boldsymbol{E}' = -\boldsymbol{E}, \qquad \boldsymbol{B}' = -\boldsymbol{B}.$$

and

$$\boldsymbol{E} = -\nabla A_0 - \frac{1}{c}\frac{\partial \boldsymbol{A}}{\partial t}, \qquad \boldsymbol{B} = \nabla \times \boldsymbol{A}$$

Then we get

$$A_k'(\boldsymbol{r}'t') = -A_k(\boldsymbol{r},t), \qquad A_4'(\boldsymbol{r}'t') = A_4(\boldsymbol{r},t).$$

Dirac equation is given by

$$(\frac{\partial}{\partial x_\mu'} - \frac{ie}{\hbar c}A_\mu')\gamma_\mu\psi' + \frac{mc}{\hbar}\psi' = 0$$

or equivalently

$$[-(\frac{\partial}{\partial x_k} - \frac{ie}{\hbar c}A_k)\gamma_k + (\frac{\partial}{\partial x_4} - \frac{ie}{\hbar c}A_4)\gamma_4]\psi' + \frac{mc}{\hbar}\psi' = 0.$$

We try as before

$$\psi' = S_p\psi$$

$$[-(\frac{\partial}{\partial x_k} - \frac{ie}{\hbar c}A_k)\gamma_k + (\frac{\partial}{\partial x_4} - \frac{ie}{\hbar c}A_4)\gamma_4]S_p\psi + \frac{mc}{\hbar}S_p\psi = 0$$

Multiplying S_p^{-1} from the left,

$$S_p^{-1}[-(\frac{\partial}{\partial x_k} - \frac{ie}{\hbar c}A_k)\gamma_k + (\frac{\partial}{\partial x_4} - \frac{ie}{\hbar c}A_4)\gamma_4]S_p\psi + \frac{mc}{\hbar}\psi = 0.$$

When this equation is compared with the original Dirac equation,

$$(\frac{\partial}{\partial x_\mu} - \frac{ie}{\hbar c}A_\mu)\gamma_\mu\psi + \frac{mc}{\hbar}\psi = 0,$$

we have

$$S_p^{-1}\gamma_k S_p\psi = -\gamma_k, \qquad S_p^{-1}\gamma_4 S_p\psi = \gamma_4$$

We assume that

$$S_p = \eta\gamma_4$$

where η is some multiplicative constant. Here we use

$$S_p = \gamma_4 = \beta = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

for an electron wave function.

7.2 Definition of the parity operator *P*

We define the parity operator as

$$P = \beta\pi$$

where β operates on the Dirac space and π operates on the coordinate space. Note that

$$P^2 = \beta\pi\beta\pi = \beta^2\pi^2 = 1$$

The commutation relation between *H* (for the free particle) and *P* is given by

$$\begin{aligned}
[P,H] &= [\beta\pi, c\alpha_k p_k + \beta mc^2] \\
&= [\beta\pi, c\alpha_k p_k] \\
&= \beta\pi c\alpha_k p_k - c\alpha_k p_k \beta\pi \\
&= c\beta\alpha_k \pi p_k - c\alpha_k \beta p_k \pi \\
&= c(\beta\alpha_k + \alpha_k\beta)\pi p_k \\
&= c\{\beta, \alpha_k\}\pi p_k \\
&= 0
\end{aligned}$$

where $\pi p_k + p_k\pi = 0$. Then the eigenket of *P* is the same as that of *H*.

What happened to the wave function?

$$|\psi'\rangle = \beta\pi|\psi\rangle;$$

$$\begin{aligned}
\psi'(\boldsymbol{r}) &= \langle \boldsymbol{r}|\psi'\rangle \\
&= \langle \boldsymbol{r}|\beta\pi|\psi\rangle \\
&= \beta\langle \boldsymbol{r}|\pi|\psi\rangle \\
&= \beta\langle -\boldsymbol{r}|\psi\rangle \\
&= \beta\psi(-\boldsymbol{r})
\end{aligned}$$

For the change in $\boldsymbol{r} \rightarrow -\boldsymbol{r}$, we have

$$\psi'(-\boldsymbol{r}) = \beta\psi(\boldsymbol{r}) = \gamma_4\psi(\boldsymbol{r})$$

When the time t is taken into account, we have

$$\psi'(\boldsymbol{r},t) = \gamma_4\psi(-\boldsymbol{r},t) .$$

7.3 Two component wave functions ψ_A and ψ_B under the parity operation

Since

$$\psi = \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix}$$

we get

$$\psi'(\boldsymbol{r},t) = \begin{pmatrix} \psi_A'(\boldsymbol{r},t) \\ \psi_B'(\boldsymbol{r},t) \end{pmatrix} = \gamma_4\psi(-\boldsymbol{r},t) = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}\begin{pmatrix} \psi_A(-\boldsymbol{r},t) \\ \psi_B(-\boldsymbol{r},t) \end{pmatrix}$$

Then we have

$$\psi_A'(\boldsymbol{r},t) = \psi_A(-\boldsymbol{r},t) \qquad \text{(the same as the non-relativistic case)}$$

$$\psi_B'(\boldsymbol{r},t) = -\psi_B(-\boldsymbol{r},t)$$

The upper and lower components of the wave functions have different behaviors under a parity transformation.

This is expected from the following discussion of Dirac equation.

$$H\psi = E\psi$$

$$\psi = \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix}, \qquad H = c\boldsymbol{\alpha}\cdot(\boldsymbol{p} - \frac{e}{c}\boldsymbol{A}) + \beta mc^2$$

Eigenvalue problem:

$$H\psi = \begin{pmatrix} mc^2 & c\boldsymbol{\sigma}\cdot(\boldsymbol{p} - \frac{e}{c}\boldsymbol{A}) \\ c\boldsymbol{\sigma}\cdot(\boldsymbol{p} - \frac{e}{c}\boldsymbol{A}) & -mc^2 \end{pmatrix}\begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix} = E\begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix}$$

Or

$$c\boldsymbol{\sigma}\cdot(\boldsymbol{p}-\frac{e}{c}\boldsymbol{A})\psi_A - mc^2\psi_B = E\psi_B$$

Then we have

$$\psi_B(\boldsymbol{r},t) = \frac{1}{E+mc^2}c\boldsymbol{\sigma}\cdot(\boldsymbol{p}-\frac{e}{c}\boldsymbol{A})\psi_A(\boldsymbol{r},t)$$

Under the parity,

$$\boldsymbol{p}\to -\boldsymbol{p}, \qquad \boldsymbol{A}\to -\boldsymbol{A},$$

$$\psi_A(\boldsymbol{r},t)\to \psi_A'(-\boldsymbol{r},t),$$

then we get

$$\begin{aligned}\psi_B'(-\mathbf{r},t) &= -\frac{1}{E+mc^2}c\boldsymbol{\sigma}\cdot(\mathbf{p}-\frac{e}{c}\mathbf{A})\psi_A'(-\mathbf{r},t)\\ &= -\frac{1}{E+mc^2}c\boldsymbol{\sigma}\cdot(\mathbf{p}-\frac{e}{c}\mathbf{A})\psi_A(\mathbf{r},t)\\ &= -\psi_B(\mathbf{r},t)\end{aligned}$$

where

$$\psi_A'(-\boldsymbol{r},t) = \psi_A(\boldsymbol{r},t)$$

7.4 Even or odd parity in ψ_A and ψ_B

Suppose that $|\psi_A\rangle$ and $|\psi_B\rangle$ has different parities (even or odd).

$$\pi|\psi_A\rangle = \pm|\psi_A\rangle, \qquad \pi|\psi_B\rangle = \mp|\psi_B\rangle$$

or

$$\langle\boldsymbol{r}|\pi|\psi_A\rangle = \langle-\boldsymbol{r}|\psi_A\rangle = \pm\langle-\boldsymbol{r}|\psi_A\rangle$$

and

$$\langle\boldsymbol{r}|\pi|\psi_B\rangle = \langle-\boldsymbol{r}|\psi_B\rangle = \mp\langle-\boldsymbol{r}|\psi_B\rangle$$

Then we get

$$\beta\psi(-\boldsymbol{r},t)=\begin{pmatrix} I_2 & 0 \\ 0 & -I_2 \end{pmatrix}\begin{pmatrix} \psi_A(-\boldsymbol{r},t) \\ \psi_B(-\boldsymbol{r},t) \end{pmatrix}=\begin{pmatrix} \psi_A(-\boldsymbol{r},t) \\ -\psi_B(-\boldsymbol{r},t) \end{pmatrix}=\pm\begin{pmatrix} \psi_A(\boldsymbol{r},t) \\ \psi_B(\boldsymbol{r},t) \end{pmatrix}=\pm\psi(\boldsymbol{r},t)$$

or, formally

$$\gamma_4\psi(-\boldsymbol{r},t)=\pm\psi(\boldsymbol{r},t).$$

since

$$\psi_A(-\boldsymbol{r},t)=\pm\psi_A(\boldsymbol{r},t), \qquad \psi_B(-\boldsymbol{r},t)=\mp\psi_B(\boldsymbol{r},t).$$

We assume that ψ_A and ψ_B are the eigenstates of the orbital angular momentum.

$$\psi_A(-\boldsymbol{r},t)=(-1)^{l_A}\psi_A(\boldsymbol{r},t)=\pm\psi_A(\boldsymbol{r},t)$$

$$\psi_B(-\boldsymbol{r},t)=(-1)^{l_B}\psi_B(\boldsymbol{r},t)=\mp\psi_B(\boldsymbol{r},t)$$

where l_A and l_B are the orbital angular momenta of the two-component wave function $\psi_A(\boldsymbol{r},t)$ and $\psi_B(\boldsymbol{r},t)$, respectively. Thus we have

$$(-1)^{l_A}=(-1)^{l_B+1}$$

This implies that if $\psi_A(\boldsymbol{r},t)$ is a two-component wave function with an even (odd) orbital angular momentum, then $\psi_B(\boldsymbol{r},t)$ is a two-component wave function with an odd (even) orbital angular momentum.

((**Example**))

We consider the case of a central force.

$$\boldsymbol{A}=0, \qquad A_0=\phi, \qquad eA_0=V(r)$$

$$\psi=\begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix}, \qquad H=c\boldsymbol{\alpha}\cdot\boldsymbol{p}+\beta mc^2+V(r)$$

$$H\psi=\begin{pmatrix} mc^2+V(r) & c\boldsymbol{\sigma}\cdot\boldsymbol{p} \\ c\boldsymbol{\sigma}\cdot\boldsymbol{p} & -mc^2+V(r) \end{pmatrix}\begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix}=E\begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix}$$

Then we get

$$\psi_B(\boldsymbol{r},t) = \frac{c}{E - V(r) + mc^2}(\boldsymbol{\sigma}\cdot\boldsymbol{p})\psi_A(\boldsymbol{r},t)$$

Let us suppose that $\psi_A(\boldsymbol{r},t)$ is an ${}^2S_{1/2}$ state wave function with spin up (l = 0, s = 1/2)

$$\psi_A(\boldsymbol{r},t) = R(r)\begin{pmatrix}1\\0\end{pmatrix}e^{-\frac{iEt}{\hbar}}$$

Then

$$\psi_B(\boldsymbol{r},t) = \frac{-i\hbar c}{E - V(r) + mc^2}\begin{pmatrix}\frac{\partial}{\partial x_3} & \frac{\partial}{\partial x_1} - i\frac{\partial}{\partial x_2}\\ \frac{\partial}{\partial x_1} + i\frac{\partial}{\partial x_2} & -\frac{\partial}{\partial x_3}\end{pmatrix}\begin{pmatrix}R(r)\\0\end{pmatrix}e^{-\frac{iEt}{\hbar}}$$

Note that

$$\frac{\partial}{\partial x_3}R(r) = \frac{\partial r}{\partial x_3}\frac{dR}{dr} = \frac{x_3}{r}\frac{dR}{dr},$$

$$\frac{\partial}{\partial x_1}R(r) == \frac{x_1}{r}\frac{dR}{dr}, \qquad \frac{\partial}{\partial x_2}R(r) == \frac{x_2}{r}\frac{dR}{dr}$$

Then we get

$$\begin{aligned}\psi_B(\boldsymbol{r},t) &= \frac{-i\hbar c}{E - V(r) + mc^2}\frac{1}{r}\frac{dR}{dr}\begin{pmatrix}x_3 & x_1 - ix_2\\ x_1 + ix_2 & -x_3\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix}e^{-\frac{iEt}{\hbar}}\\ &= \frac{-i\hbar c}{E - V(r) + mc^2}\frac{1}{r}\frac{dR}{dr}\begin{pmatrix}x_3\\ x_1 + ix_2\end{pmatrix}e^{-\frac{iEt}{\hbar}}\\ &= \frac{-i\hbar c}{E - V(r) + mc^2}\frac{1}{r}\frac{dR}{dr}[x_3\begin{pmatrix}1\\0\end{pmatrix} + (x_1 + ix_2)\begin{pmatrix}0\\1\end{pmatrix}]e^{-\frac{iEt}{\hbar}}\end{aligned}$$

Here we note that

$$Y_1^1 = \frac{1}{2}\sqrt{\frac{3}{2\pi}}\sin\theta e^{i\phi} = \frac{1}{2}\sqrt{\frac{3}{2\pi}}\frac{x_1 + ix_2}{r}$$

$$Y_1^0 = \frac{1}{2}\sqrt{\frac{3}{\pi}}\cos\theta = \sqrt{\frac{3}{4\pi}}\frac{x_3}{r}$$

$$Y_1^{-1} = \frac{1}{2}\sqrt{\frac{3}{2\pi}}\sin\theta e^{-i\phi} = \frac{1}{2}\sqrt{\frac{3}{2\pi}}\frac{x_1 - ix_2}{r}$$

where

$$x_1 = \sin\theta\cos\phi, \qquad x_2 = \sin\theta\sin\phi, \qquad x_3 = \cos\theta$$

Thus we have

$$\psi_B(\boldsymbol{r},t) = \frac{-i\hbar c}{E - V(r) + mc^2}\frac{dR}{dr}[\sqrt{\frac{4\pi}{3}}Y_1^0\begin{pmatrix}1\\0\end{pmatrix} + \sqrt{\frac{8\pi}{3}}Y_1^1\begin{pmatrix}0\\1\end{pmatrix}]e^{-\frac{iEt}{\hbar}}$$

The first term of the parenthesis is $l = 1$ and $s = 1/2$
$j = 1/2$ $({}^2P_{1/2})$

The second term of the parenthesis is $l = 1$ and $s = 1/2$
$j = 3/2$ $({}^2P_{3/2})$
$j = 1/2$ $({}^2P_{1/2})$

((Note)) Parity operator π in non-relativistic quantum mechanics

$$|\psi'\rangle = \hat{\pi}|\psi\rangle \quad \text{with} \quad \hat{\pi}^+\hat{\pi} = \hat{1} \text{ and } \hat{\pi}^+ = \hat{\pi}$$

$$\langle\psi'|\hat{x}|\psi'\rangle = -\langle\psi|\hat{x}|\psi\rangle, \qquad \hat{\pi}^+\hat{x}\hat{\pi} = -\hat{x}$$

$$\hat{\pi}|x\rangle = |-x\rangle$$

$$\langle x|\psi'\rangle = \langle x|\hat{\pi}|\psi\rangle, \quad \text{or} \quad \psi'(x) = \psi(-x)$$

Even parity: $\langle x|\psi'\rangle = \langle x|\hat{\pi}|\psi\rangle = \langle x|\psi\rangle$, $\psi'(x) = \psi(-x) = \psi(x)$

Odd parity $\langle x|\hat{\pi}|\psi\rangle = -\langle x|\psi\rangle$, $\psi'(x) = \psi(-x) = -\psi(x)$

---

8. Eigenvalue problem (degenerate case)

We solve the eigenvalue problem using the Mathematica.

$$H - EI_4 = \begin{pmatrix} mc^2 - E & 0 & cp_z & c(p_x - ip_y) \\ 0 & mc^2 - E & c(p_x + ip_y) & -cp_z \\ cp_z & c(p_x - ip_y) & -mc^2 - E & 0 \\ c(p_x + ip_y) & -cp_z & 0 & -mc^2 - E \end{pmatrix}$$

From the condition that det($H - \varepsilon I_4$)=0, we get

$$E = \pm R = \pm\sqrt{m^2c^4 + c^2\boldsymbol{p}^2}$$

where

$$R = \sqrt{m^2c^4 + c^2\boldsymbol{p}^2} \quad (>0)$$

Thus we see that there are four eigenvalues which are degenerate in pairs, i.e.

E = +R, +R, -R, and -R

For simplicity we assume that

$$p_x = p_y = 0$$

For E = +R

$$\begin{pmatrix} mc^2 - R & 0 & cp_z & 0 \\ 0 & mc^2 - R & 0 & -cp_z \\ cp_z & 0 & -mc^2 - R & 0 \\ 0 & -cp_z & 0 & -mc^2 - R \end{pmatrix}\begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

or

$$\begin{aligned} &(mc^2 - R)u_1 + cp_z u_3 = 0 \\ &(mc^2 - R)u_2 - cp_z u_4 = 0 \\ &cp_z u_1 - (R + mc^2)u_3 = 0 \\ &-cp_z u_2 - (mc^2 + R)u_4 = 0 \end{aligned}$$

It is clear from the above equations that at the zero momentum limit ($p_z \to 0$) the first two equations do not give us any information on the unknowns. Thus we need to solve the second two equations. The two independent solutions, corresponding to the eigenvalue $+R$,

$$u_1 = 1,\ u_2 = 0,\ u_3 = \frac{cp_z}{R + mc^2},\ u_4 = 0.$$

$$u_1 = 0,\ u_2 = 1,\ u_3 = 0,\ u_4 = -\frac{cp_z}{R + mc^2}.$$

For $E = -R$

$$\begin{pmatrix} mc^2 + R & 0 & cp_z & 0 \\ 0 & mc^2 + R & 0 & -cp_z \\ cp_z & 0 & -mc^2 + R & 0 \\ 0 & -cp_z & 0 & -mc^2 + R \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

or

$$\begin{aligned} &(mc^2 + R)u_1 + cp_z u_3 = 0 \\ &(mc^2 + R)u_2 - cp_z u_4 = 0 \\ &cp_z u_1 - (R - mc^2)u_3 = 0 \\ &-cp_z u_2 - (mc^2 - R)u_4 = 0 \end{aligned}$$

It is clear from the above equations that at the zero momentum limit ($p_z \rightarrow 0$) the second two equations do not give us any information on the unknowns. Thus we need to solve the first two equations. The two independent solutions, corresponding to the eigenvalue -R,

$$u_1 = -\frac{cp_z}{R + mc^2},\ u_2 = 0,\ u_3 = 1, ,\ u_4 = 0.$$

$$u_1 = 0,\ u_2 = \frac{cp_z}{R + mc^2},\ u_3 = 0,\ u_4 = 1.$$

((Summary))

For $E = R$ (positive energy)

$$\sqrt{\frac{R+mc^2}{2R}}\begin{pmatrix} 1 \\ 0 \\ \frac{cp_z}{R+mc^2} \\ 0 \end{pmatrix} \qquad \sqrt{\frac{R+mc^2}{2R}}\begin{pmatrix} 0 \\ 1 \\ 0 \\ -\frac{cp_z}{R+mc^2} \end{pmatrix},$$

For $E=-R$ (negative energy)

$$\sqrt{\frac{R+mc^2}{2R}}\begin{pmatrix} \frac{-cp_z}{R+mc^2} \\ 0 \\ 1 \\ 0 \end{pmatrix} \qquad \sqrt{\frac{R+mc^2}{2R}}\begin{pmatrix} 0 \\ \frac{cp_z}{R+mc^2} \\ 0 \\ 1 \end{pmatrix}$$

If $p_z = 0$, we have

$$\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \qquad \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix},$$

The non-relativistic spin sttes. These are degenerate and have energy eigenvalue +R.

$$\begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \qquad \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

The nonrelativistic spin states. These are degenerate and have energy eigenvlaue -R.

9. The use of the Mathematica to derive the eigenkets of *H*

The eigenvalue problem can be solved Using the Eigensystem[*H*] of the Mathematica,.

((Mathematica))

```
Clear["Global`*"]; exp_* := exp /. {Complex[re_, im_] :> Complex[re, -im]};
σx = (0 1
      1 0); σy = (0 -ⅈ
                  ⅈ  0); σz = (1  0
                               0 -1);
I2 = IdentityMatrix[2]; I4 = IdentityMatrix[4];
αx = KroneckerProduct[σx, σx]; αy = KroneckerProduct[σx, σy];
αz = KroneckerProduct[σx, σz]; β = KroneckerProduct[σz, I2];
H = m c^2 β + c (αx px + αy py + αz pz);
rule1 = {Sqrt[c^2 m^2 + (px^2 + py^2 + pz^2)] -> R/c};
rule2 = {(px^2 + py^2 + pz^2) -> R^2/c^2 - c^2 m^2};
rule3 = {R -> c Sqrt[c^2 m^2 + px^2 + py^2 + pz^2]};
```

Eigenvalue problem of the Hamiltonian of the Dirac free particle

```
eq1 = Eigensystem[H] /. rule1 // FullSimplify
```

$$\left\{\{-R, -R, R, R\}, \left\{\left\{-\frac{c\,(px - i\,py)}{c^2 m + R}, \frac{c\,pz}{c^2 m + R}, 0, 1\right\}, \left\{-\frac{c\,pz}{c^2 m + R}, -\frac{c\,(px + i\,py)}{c^2 m + R}, 1, 0\right\}, \left\{\frac{c\,(px - i\,py)}{-c^2 m + R}, \frac{c\,pz}{c^2 m - R}, 0, 1\right\}, \left\{\frac{c\,pz}{-c^2 m + R}, \frac{c\,(px + i\,py)}{-c^2 m + R}, 1, 0\right\}\right\}\right\}$$

Orthogonality

```
eq1[[2, 1]]*.eq1[[2, 2]] /. rule3 // Simplify
```

0

```
eq1[[2, 1]]*.eq1[[2, 3]] /. rule3 // Simplify
```

0

```
eq1[[2, 1]]*.eq1[[2, 4]] /. rule3 // Simplify
```

0

```
eq1[[2, 2]]*.eq1[[2, 3]] /. rule3 // Simplify
```

0

```
eq1[[2, 2]]*.eq1[[2, 4]] /. rule3 // Simplify
```

0

```
eq1[[2, 3]]*.eq1[[2, 4]] /. rule3 // Simplify
```

```
0
```

Normalization constant

```
A1 = eq1[[2, 1]]*.eq1[[2, 1]] // Simplify; A11 = A1 /. rule2 // Simplify
```

$$\frac{2R}{c^2 m + R}$$

```
A2 = eq1[[2, 2]]*.eq1[[2, 2]] // Simplify; A21 = A2 /. rule2 // Simplify
```

$$\frac{2R}{c^2 m + R}$$

```
A3 = eq1[[2, 3]]*.eq1[[2, 3]] // Simplify; A31 = A3 /. rule2 // Simplify
```

$$-\frac{2R}{c^2 m - R}$$

```
A4 = eq1[[2, 4]]*.eq1[[2, 4]] // Simplify; A41 = A4 /. rule2 // Simplify
```

$$-\frac{2R}{c^2 m - R}$$

The results are as follows.

For $E = R$ (positive energy)

$$\sqrt{\frac{R-mc^2}{2R}}\begin{pmatrix} \dfrac{cp_z}{R-mc^2} \\ \dfrac{c(p_x+ip_y)}{R-mc^2} \\ 1 \\ 0 \end{pmatrix} \qquad \sqrt{\frac{R-mc^2}{2R}}\begin{pmatrix} \dfrac{c(p_x-ip_y)}{R-mc^2} \\ \dfrac{-cp_z}{R-mc^2} \\ 1 \\ 0 \end{pmatrix},$$

For $E = -R$ (negative energy)

$$\sqrt{\frac{R+mc^2}{2R}}\begin{pmatrix} \dfrac{-cp_z}{R+mc^2} \\ \dfrac{-c(p_x+ip_y)}{R+mc^2} \\ 1 \\ 0 \end{pmatrix} \qquad \sqrt{\frac{R+mc^2}{2R}}\begin{pmatrix} \dfrac{-c(p_x-ip_y)}{R+mc^2} \\ \dfrac{cp_z}{R+mc^2} \\ 0 \\ 1 \end{pmatrix}$$

10. Conserved current

$$\psi = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix}$$

$$\psi^+ = \left(\psi^*{}_1 \quad \psi_2{}^* \quad \psi_3{}^* \quad \psi_4{}^*\right)$$

$$\begin{aligned} \overline{\psi} &= \left(\psi^*{}_1 \quad \psi_2{}^* \quad -\psi_3{}^* \quad -\psi_4{}^*\right) \\ &= \psi^+\gamma_4 \\ &= \left(\psi^*{}_1 \quad \psi_2{}^* \quad \psi_3{}^* \quad \psi_4{}^*\right)\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \end{aligned}$$

In order to obtain the wave equation for $\overline{\psi}$, we start from the Dirac equation

$$[\boldsymbol{\gamma}\cdot\nabla + \gamma_4 \frac{\partial}{\partial(ix_0)} + \frac{mc}{\hbar}]\psi = 0$$

or

$$(\gamma_k \frac{\partial}{\partial x_k} + \gamma_4 \frac{\partial}{\partial x_4} + \frac{mc}{\hbar})\psi = 0 \qquad (k = 1, 2, 3).$$

or

$$(\gamma_\mu \frac{\partial}{\partial x_\mu} + \frac{mc}{\hbar})\psi = 0 \qquad (\mu = 1, 2, 3, 4).$$

where $x_1 = x$, $x_2 = y$, $x_3 = z$, $x_4 = \mathrm{i}x_0 = \mathrm{i}ct$

We take the hermitian conjugate of the Dirac equation,

$$\frac{\partial}{\partial x_k}\psi^+\gamma_k + \frac{\partial}{\partial x_4{}^*}\psi^+\gamma_4 + \frac{mc}{\hbar}\psi^+ = 0 \qquad (1)$$

Multiplying Eq.(1) by γ_4 from the right, we get

$$\frac{\partial}{\partial x_k}\psi^+\gamma_k\gamma_4 + \frac{\partial}{\partial x_4{}^*}\psi^+\gamma_4{}^2 + \frac{mc}{\hbar}\psi^+\gamma_4 = 0\,.$$

Since $\gamma_4\gamma_k = -\gamma_k\gamma_4$, we have

$$-\frac{\partial}{\partial x_k}\psi^+\gamma_4\gamma_k - \frac{\partial}{\partial x_4}\psi^+\gamma_4{}^2 + \frac{mc}{\hbar}\psi^+\gamma_4 = 0$$

or

$$-\frac{\partial}{\partial x_\mu}\psi^+\gamma_4\gamma_\mu + \frac{mc}{\hbar}\psi^+\gamma_4 = 0$$

or

$$(-\frac{\partial}{\partial x_\mu}\overline{\psi})\gamma_\mu + \frac{mc}{\hbar}\overline{\psi} = 0$$

Now we have

$$(\gamma_\mu\frac{\partial}{\partial x_\mu} + \frac{mc}{\hbar})\psi = 0 \tag{2}$$

and

$$(-\frac{\partial}{\partial x_\mu}\overline{\psi})\gamma_\mu + \frac{mc}{\hbar}\overline{\psi} = 0 \tag{3}$$

$\overline{\psi}$ x Eq.(2) leads to

$$\overline{\psi}(\gamma_\mu\frac{\partial}{\partial x_\mu} + \frac{mc}{\hbar})\psi = 0 \tag{2'}$$

Eq.(3) x ψ leads to

$$(-\frac{\partial}{\partial x_\mu}\overline{\psi})\gamma_\mu + \frac{mc}{\hbar}\overline{\psi})\psi = 0 \tag{3'}$$

The subtraction of Eq.(3') from Eq.(2') yields

$$\overline{\psi}\gamma_\mu\frac{\partial}{\partial x_\mu}\psi + (\frac{\partial}{\partial x_\mu}\overline{\psi})\gamma_\mu\psi = 0\,.$$

or

$$\frac{\partial}{\partial x_\mu}(\overline{\psi}\gamma_\mu\psi) = 0$$

Thus we see that

$$S_\mu = ic\,\overline{\psi}\gamma_\mu\psi = (c\,\overline{\psi}\alpha_k\psi\,, ic\,\psi^+\psi)$$

$$\frac{\partial}{\partial x_\mu}S_\mu = 0$$

or

$$\nabla\cdot\boldsymbol{S} + \frac{\partial}{\partial(ict)}ic\psi^+\psi = 0$$

or

$$\frac{\partial}{\partial t}\psi^+\psi + \nabla\cdot\boldsymbol{S} = 0$$

The flux density $\boldsymbol{S}$ is defined by

$$S_k = ic\overline{\psi}\gamma_k\psi = c\psi^+\alpha_k\psi$$

The probability density is defined by

$$\rho = \psi^+\psi$$

((**Note**))

$$ic\overline{\psi}\gamma_k\psi = ic\psi^+\gamma_4\gamma_k\psi = c\psi^+\alpha_k\psi = S_k$$

$$ic\overline{\psi}\gamma_4\psi = ic\psi^+\gamma_4\gamma_4\psi = ic\psi^+\psi$$

where

$$\alpha_k = i\gamma_4\gamma_k$$

11. Simple solutions: nonrelativistic approximation

In the presence of electromagnetic fields,

$$p_\mu = \frac{\hbar}{i}\frac{\partial}{\partial x_\mu} \to p_\mu - \frac{e}{c}A_\mu$$

or

$$\frac{\partial}{\partial x_\mu} \to \frac{i}{\hbar}(p_\mu - \frac{e}{c}A_\mu)$$

Dirac equation

$$(\gamma_\mu \frac{\partial}{\partial x_\mu} + \frac{mc}{\hbar})\psi = 0 \to [\gamma_\mu \frac{i}{\hbar}(p_\mu - \frac{e}{c}A_\mu) + \frac{mc}{\hbar}]\psi = 0$$

or

$$[\gamma_\mu (p_\mu - \frac{e}{c}A_\mu) - imc]\psi = 0$$

or

$$\left\{ \begin{pmatrix} 0 & -i\boldsymbol{\sigma} \\ i\boldsymbol{\sigma} & 0 \end{pmatrix} (\boldsymbol{p} - \frac{e}{c}\boldsymbol{A}) + \begin{pmatrix} \boldsymbol{I} & 0 \\ 0 & -\boldsymbol{I} \end{pmatrix} (p_4 - \frac{e}{c}A_4) - imc \right\} \psi = 0$$

or

$$\begin{pmatrix} 0 & -i\boldsymbol{\sigma}\cdot(\boldsymbol{p} - \frac{e}{c}\boldsymbol{A}) \\ i\boldsymbol{\sigma}\cdot(\boldsymbol{p} - \frac{e}{c}\boldsymbol{A}) & 0 \end{pmatrix} \psi + \begin{pmatrix} p_4 - \frac{e}{c}A_4 & 0 \\ 0 & -(p_4 - \frac{e}{c}A_4) \end{pmatrix} \psi = imc\psi$$

Noting that $A_4 = iA_0$ and $p_4 = \frac{\hbar}{i}\frac{\partial}{\partial x_4} = -\frac{\hbar}{c}\frac{\partial}{\partial t}$

$$\begin{pmatrix} 0 & -i\sigma\cdot(\boldsymbol{p} - \frac{e}{c}\boldsymbol{A}) \\ i\sigma\cdot(\boldsymbol{p} - \frac{e}{c}\boldsymbol{A}) & 0 \end{pmatrix} \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix} + \begin{pmatrix} -\frac{\hbar}{c}\frac{\partial}{\partial t} - \frac{ie}{c}A_0 & 0 \\ 0 & \frac{\hbar}{c}\frac{\partial}{\partial t} + \frac{ie}{c}A_0) \end{pmatrix} \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix} = imc \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix}$$

or

$$-i\boldsymbol{\sigma}\cdot(\boldsymbol{p}-\frac{e}{c}\boldsymbol{A})\psi_B-\frac{i}{c}(-i\hbar\frac{\partial}{\partial t}+eA_0)\psi_A=imc\psi_A$$

$$i\boldsymbol{\sigma}\cdot(\boldsymbol{p}-\frac{e}{c}\boldsymbol{A})\psi_A+\frac{i}{c}(-i\hbar\frac{\partial}{\partial t}+eA_0)\psi_B=imc\psi_B$$

or

$$\boldsymbol{\sigma}\cdot(\boldsymbol{p}-\frac{e}{c}\boldsymbol{A})\psi_B=\frac{1}{c}(i\hbar\frac{\partial}{\partial t}-eA_0-mc^2)\psi_A$$

$$-\boldsymbol{\sigma}\cdot(\boldsymbol{p}-\frac{e}{c}\boldsymbol{A})\psi_A=\frac{1}{c}(-i\hbar\frac{\partial}{\partial t}+eA_0-mc^2)\psi_B$$

Assuming that

$$\psi=\psi_0 e^{-iEt/\hbar}$$

$$i\hbar\frac{\partial}{\partial t}\psi_A=E\psi_A \qquad \text{or} \qquad \frac{\partial}{\partial t}\psi_A=-\frac{iE}{\hbar}\psi_A$$

$$i\hbar\frac{\partial}{\partial t}\psi_B=E\psi_B \qquad \text{or} \qquad \frac{\partial}{\partial t}\psi_B=-\frac{iE}{\hbar}\psi_B$$

Then we have

$$\boldsymbol{\sigma}\cdot(\mathbf{p}-\frac{e}{c}\mathbf{A})\psi_B=\frac{1}{c}(E-eA_0-mc^2)\psi_A$$

$$-\boldsymbol{\sigma}\cdot(\mathbf{p}-\frac{e}{c}\mathbf{A})\psi_A=-\frac{1}{c}(E-eA_0+mc^2)\psi_B$$

((Note)) A_μ is time-independent.

$$\psi_B=\frac{c}{E-eA_0+mc^2}[\sigma\cdot(\mathbf{p}-\frac{e}{c}\mathbf{A})]\psi_A$$

Substitution of this eq. into the first equation

$$[\sigma\cdot(\mathbf{p}-\frac{e}{c}\mathbf{A})]\frac{c}{E-eA_0+mc^2}[\sigma\cdot(\mathbf{p}-\frac{e}{c}\mathbf{A})]\psi_A=\frac{1}{c}(E-eA_0-mc^2)\psi_A$$

We now assume that $E \approx mc^2$ and $|eA_0| << mc^2$.

Defining the energy measured from mc^2,

$$E^{(NR)} = E - mc^2$$

$$\begin{aligned}
\frac{c}{E - eA_0 + mc^2} &= \frac{1}{2m}\left(\frac{2mc^2}{2mc^2 + E^{(NR)} - eA_0}\right) \\
&= \frac{1}{2m}\frac{1}{1+\dfrac{E^{(NR)} - eA_0}{2mc^2}} \\
&= \frac{1}{2m}[1 - (\frac{E^{(NR)} - eA_0}{2mc^2}) + ...] \\
&= \frac{1}{2m}
\end{aligned}$$

$$\frac{1}{2m}[\boldsymbol{\sigma}\cdot(\mathbf{p} - \frac{e}{c}\mathbf{A})][\boldsymbol{\sigma}\cdot(\mathbf{p} - \frac{e}{c}\mathbf{A})]\psi_A = (E^{(NR)} - eA_0)\psi_A$$

which becomes

$$[\frac{1}{2m}(\boldsymbol{p} - \frac{e}{c}\boldsymbol{A})^2 - \frac{e\hbar}{2mc}\boldsymbol{\sigma}\cdot\boldsymbol{B} + eA_0]\psi_A = E^{(NR)}\psi_A$$

((**Note**))

$$\begin{aligned}
[\boldsymbol{\sigma}\cdot(\boldsymbol{p} - \frac{e}{c}\boldsymbol{A})][\boldsymbol{\sigma}\cdot(\boldsymbol{p} - \frac{e}{c}\boldsymbol{A})] &= (\boldsymbol{p} - \frac{e}{c}\boldsymbol{A})^2 + i\boldsymbol{\sigma}\cdot[(\boldsymbol{p} - \frac{e}{c}\boldsymbol{A})\times(\boldsymbol{p} - \frac{e}{c}\boldsymbol{A})] \\
&= (\boldsymbol{p} - \frac{e}{c}\boldsymbol{A})^2 - \frac{e\hbar}{c}\boldsymbol{\sigma}\cdot B
\end{aligned}$$

since

$$\begin{aligned}
(\boldsymbol{p} - \frac{e}{c}\boldsymbol{A})\times(\boldsymbol{p} - \frac{e}{c}\boldsymbol{A}) &= -\frac{e}{c}(\boldsymbol{p}\times\boldsymbol{A} + \boldsymbol{A}\times\boldsymbol{P}) \\
&= \frac{ie\hbar}{c}\nabla\times\boldsymbol{A} \\
&= \frac{ie\hbar}{c}\boldsymbol{B}
\end{aligned}$$

((**Comment**))

To zeroth order in $(v/c)^2$, ψ_A is nothing more than the Schrödinger-Pauli two component wave function in nonrelativistic quantum mechanics, multiplied by $\exp(-imc^2 t/\hbar)$.

ψ_B is "smaller" than ψ_A by a factor of roughly $\left|\boldsymbol{p} - e\boldsymbol{A}/c\right|/2mc \approx v/(2c)$ if $E \approx mc^2$ and $\left|eA_0\right| << mc^2$.

For this reason with mc^2, ψ_A and ψ_B are known as the large and small components of the Dirac wave function ψ.

Since

$$-\boldsymbol{\sigma}\cdot(\boldsymbol{p} - \frac{e}{c}\boldsymbol{A})\psi_A = -\frac{1}{c}(E - eA_0 + mc^2)\psi_B = -2mc\psi_B$$

$$\psi_B = \frac{1}{2mc}\boldsymbol{\sigma}\cdot(\boldsymbol{p} - \frac{e}{c}\boldsymbol{A})\psi_A$$

12. Approximate Hamiltonian for an electrostatic problem

$$[\boldsymbol{\sigma}\cdot(\boldsymbol{p} - \frac{e}{c}\boldsymbol{A})]\frac{c^2}{E - eA_0 + mc^2}[\boldsymbol{\sigma}\cdot(\boldsymbol{p} - \frac{e}{c}\boldsymbol{A})]\psi_A = (E - eA_0 - mc^2)\psi_A$$

For simplicity $\boldsymbol{A} = 0$.

$$\frac{1}{2m}(\boldsymbol{\sigma}\cdot\boldsymbol{p})[1 - \frac{E^{(NR)} - eA_0}{2mc^2}](\boldsymbol{\sigma}\cdot\boldsymbol{p})\psi_A = (E^{(NR)} - eA_0)\psi_A$$

or

$$H_A^{(NR)}\psi_A = E^{(NR)}\psi_A$$

with

$$H_A^{(NR)} = \frac{1}{2m}(\boldsymbol{\sigma}\cdot\boldsymbol{p})[1 - (\frac{E^{(NR)} - eA_0}{2mc^2})](\boldsymbol{\sigma}\cdot\boldsymbol{p}) + eA_0 \qquad (1)$$

It might appear that Eq.(1) is the time-independent Schrödinger equation.

However, there are three difficulities with this interpretation.

(1) Normalization

$$\int (\psi_A{}^+\psi_A + \psi_B{}^+\psi_B) d^3x = 1$$

(2) $H_A^{(NR)}$ contains a non-Hermitian term ($i\hbar\mathbf{E}\cdot\mathbf{p}$)

(3) Since $H_A^{(NR)}$ contains $E^{(NR)}$ itself, Eq.(1) is not an eigenvalue equation.

Since

$$\psi_B = \frac{1}{2mc}(\boldsymbol{\sigma}\cdot\boldsymbol{p})\psi_A$$

$$\psi_B{}^+ = \psi_A{}^+\frac{1}{2mc}(\boldsymbol{\sigma}\cdot\boldsymbol{p})$$

Normalization:

$$\int (\psi_A{}^+\psi_A + \frac{1}{4m^2c^2}\psi_B{}^+(\sigma\cdot\mathbf{p})\psi_A) d^3x = 1$$

to order $(v/c)^2$.

This suggests that we should work wit a new-two component wave function Ψ defined by

$$\Psi = \Omega\psi_A$$

or

$$\psi_A = \Omega^{-1}\Psi$$

where

$$\Omega = 1 + \frac{\mathbf{p}^2}{8m^2c^2}$$

With this choice

$$\begin{aligned}\int \Psi^+\Psi d^3x &\approx \int (\psi_A{}^+(1+\frac{\boldsymbol{p}^2}{8m^2c^2})^2\psi_A d^3x \\ &= \int (\psi_A{}^+(1+\frac{\boldsymbol{p}^2}{4m^2c^2})\psi_A d^3x \\ &= 1\end{aligned}$$

$$H_A^{(NR)}\psi_A = E^{(NR)}\psi_A$$

$$H_A^{(NR)}\Omega^{-1}\Psi = E^{(NR)}\Omega^{-1}\Psi$$

or

$$\Omega^{-1}H_A^{(NR)}\Omega^{-1}\Psi = E^{(NR)}\Omega^{-2}\Psi$$

$$\begin{aligned}\Omega^{-1}H_A^{(NR)}\Omega^{-1} &= (1-\frac{\boldsymbol{p}^2}{8m^2c^2})H_A^{(NR)}(1-\frac{\boldsymbol{p}^2}{8m^2c^2}) \\ &= (H_A^{(NR)} - \frac{\boldsymbol{p}^2}{8m^2c^2}H_A^{(NR)})(1-\frac{\boldsymbol{p}^2}{8m^2c^2}) \\ &= H_A^{(NR)} - \{\frac{\boldsymbol{p}^2}{8m^2c^2}, H_A^{(NR)}\} \\ &= H_A^{(NR)} - \{\frac{\boldsymbol{p}^2}{8m^2c^2}, \frac{1}{2m}\boldsymbol{p}^2 + eA_0\}\end{aligned}$$

where

$$H_A^{(NR)} = \frac{1}{2m}\boldsymbol{p}^2 + eA_0 - \frac{1}{2m}(\boldsymbol{\sigma}\cdot\boldsymbol{p})(\frac{E^{(NR)}-eA_0}{2mc^2})](\boldsymbol{\sigma}\cdot\boldsymbol{p})$$

$$E^{(NR)}\Omega^{-2}\Psi = E^{(NR)}(1-\frac{\mathbf{p}^2}{4m^2c^2})\Psi$$

Thus we have

$$\begin{aligned}&[\frac{1}{2m}\boldsymbol{p}^2 + eA_0 - \{\frac{\boldsymbol{p}^2}{8m^2c^2}, \frac{1}{2m}\boldsymbol{p}^2 + eA_0\} \\ &-\frac{1}{2m}(\boldsymbol{\sigma}\cdot\boldsymbol{p})(\frac{E^{(NR)}-eA_0}{2mc^2})](\boldsymbol{\sigma}\cdot\boldsymbol{p})]\Psi = E^{(NR)}(1-\frac{\boldsymbol{p}^2}{4m^2c^2})\Psi\end{aligned}$$

Note

$$-\{\frac{\boldsymbol{p}^2}{8m^2c^2}, \frac{1}{2m}\boldsymbol{p}^2 + eA_0\} + E^{(NR)}\frac{\boldsymbol{p}^2}{4m^2c^2} = -\frac{\boldsymbol{p}^4}{8m^2c^2} + \frac{1}{8m^2c^2}\{\boldsymbol{p}^2, E^{(NR)} - eA_0\}$$

Then we have

$$[\frac{1}{2m}\boldsymbol{p}^2 + eA_0 - \frac{\boldsymbol{p}^4}{8m^2c^2} + \frac{1}{8m^2c^2}[\{\boldsymbol{p}^2, E^{(NR)} - eA_0\} - 2(\boldsymbol{\sigma}\cdot\boldsymbol{p})(E^{(NR)} - eA_0)](\boldsymbol{\sigma}\cdot\boldsymbol{p})]\Psi = E^{(NR)}\Psi$$

Here we use the formula

$$\{A^2, B\} = 2ABA + [A,[A,B]]$$

When

$$A = \boldsymbol{\sigma}\cdot\boldsymbol{p}\,, \qquad B = E^{(NR)} - eA_0$$

$$A^2 = (\boldsymbol{\sigma}\cdot\boldsymbol{p})(\boldsymbol{\sigma}\cdot\boldsymbol{p}) = \boldsymbol{p}^2$$

Thus we have

$$\begin{aligned}\{\boldsymbol{p}^2, E^{(NR)} - eA_0\} &= 2(\boldsymbol{\sigma}\cdot\boldsymbol{p})(E^{(NR)} - eA_0)(\boldsymbol{\sigma}\cdot\boldsymbol{p}) \\ &\quad + [(\boldsymbol{\sigma}\cdot\boldsymbol{p}),[(\boldsymbol{\sigma}\cdot\boldsymbol{p}), E^{(NR)} - eA_0]]\end{aligned}$$

or

$$\{\boldsymbol{p}^2, E^{(NR)} - eA_0\} - 2(\boldsymbol{\sigma}\cdot\boldsymbol{p})(E^{(NR)} - eA_0)(\boldsymbol{\sigma}\cdot\boldsymbol{p}) = [(\boldsymbol{\sigma}\cdot\boldsymbol{p}),[(\boldsymbol{\sigma}\cdot\boldsymbol{p}), E^{(NR)} - eA_0]]$$

Here

$$\begin{aligned}[(\boldsymbol{\sigma}\cdot\boldsymbol{p}), E^{(NR)} - eA_0] &= [(\boldsymbol{\sigma}\cdot\boldsymbol{p}), -eA_0] \\ &= -e\{(\boldsymbol{\sigma}\cdot\boldsymbol{p})A_0 - A_0(\boldsymbol{\sigma}\cdot\boldsymbol{p})\} \\ &= -e\boldsymbol{\sigma}\cdot[\boldsymbol{p}, A_0] \\ &= -e\boldsymbol{\sigma}\cdot\frac{\hbar}{i}\nabla A_0 \\ &= -ie\hbar\boldsymbol{\sigma}\cdot\boldsymbol{E}\end{aligned}$$

Note that $A_0\sigma = \sigma A_0$

$$\begin{aligned}[(\boldsymbol{\sigma}\cdot\boldsymbol{p}),[(\boldsymbol{\sigma}\cdot\boldsymbol{p}), E^{(NR)} - eA_0]] &= [(\boldsymbol{\sigma}\cdot\boldsymbol{p}), -ie\hbar(\boldsymbol{\sigma}\cdot\boldsymbol{E})] \\ &= -ie\hbar[(\boldsymbol{\sigma}\cdot\boldsymbol{p}),(\boldsymbol{\sigma}\cdot\boldsymbol{E})] \\ &= -ie\hbar[(\sigma\cdot\boldsymbol{p})(\sigma\cdot\boldsymbol{E}) - (\sigma\cdot\boldsymbol{E})(\sigma\cdot\boldsymbol{p})]\end{aligned}$$

Note that

$$(\boldsymbol{\sigma}\cdot\boldsymbol{p})(\boldsymbol{\sigma}\cdot\boldsymbol{E}) = \boldsymbol{p}\cdot\boldsymbol{E} + i\boldsymbol{\sigma}\cdot(\boldsymbol{p}\times\boldsymbol{E})$$

and

$$(\boldsymbol{\sigma}\cdot\boldsymbol{E})(\boldsymbol{\sigma}\cdot\boldsymbol{p}) = \boldsymbol{E}\cdot\boldsymbol{p} + i\boldsymbol{\sigma}\cdot(\boldsymbol{E}\times\boldsymbol{p})$$

Then we have

$$(\boldsymbol{\sigma}\cdot\boldsymbol{p})(\boldsymbol{\sigma}\cdot\boldsymbol{E})-(\boldsymbol{\sigma}\cdot\boldsymbol{E})(\boldsymbol{\sigma}\cdot\boldsymbol{p})=\frac{\hbar}{i}\nabla\cdot\boldsymbol{E}-2i\boldsymbol{\sigma}\cdot(\boldsymbol{E}\times\boldsymbol{p})$$

Finally we obtain

$$\{\frac{1}{2m}\boldsymbol{p}^2+eA_0-\frac{\boldsymbol{p}^4}{8m^2c^2}+\frac{1}{8m^2c^2}(-ie\hbar)[\frac{\hbar}{i}\nabla\cdot\boldsymbol{E}-2i\boldsymbol{\sigma}\cdot(\boldsymbol{E}\times\boldsymbol{p})]\}\Psi=E^{(NR)}\Psi$$

or

$$[\frac{1}{2m}\boldsymbol{p}^2+eA_0-\frac{\boldsymbol{p}^4}{8m^2c^2}-\frac{e\hbar}{4m^2c^2}\boldsymbol{\sigma}\cdot(\boldsymbol{E}\times\boldsymbol{p})-\frac{e\hbar^2}{8m^2c^2}\nabla\cdot\boldsymbol{E}]\Psi=E^{(NR)}\Psi$$

((Physical meaning))

Third term: relativistic correction

$$\begin{aligned}\sqrt{m^2c^4+\boldsymbol{p}^2c^2}-mc^2&=mc^2\sqrt{1+\frac{\boldsymbol{p}^2}{m^2c^2}}-mc^2\\&=mc^2[1+\frac{\boldsymbol{p}^2}{2m^2c^2}-\frac{1}{8}\frac{\boldsymbol{p}^4}{m^4c^4}+...]-mc^2\\&=\frac{\boldsymbol{p}^2}{2m}-\frac{1}{8}\frac{\boldsymbol{p}^4}{m^3c^2}+...\end{aligned}$$

The fourth term (Thomas correction)

$$\text{Thomas term}=-\frac{e\hbar}{4m^2c^2}\boldsymbol{\sigma}\cdot(\boldsymbol{E}\times\boldsymbol{p})$$

For a central potential

$$eA_0=V(r)$$

$$\boldsymbol{E}=-\nabla A_0=-\frac{1}{r}\frac{dV}{dr}\boldsymbol{r}$$

$$\boldsymbol{E}\times\boldsymbol{p}=-\frac{1}{r}\frac{dV}{dr}(\boldsymbol{r}\times\boldsymbol{p})=-\frac{1}{r}\frac{dV}{dr}\boldsymbol{L}$$

where $\boldsymbol{L}$ is an orbital angular momentum. Then the Thomas term is rewritten as

Thomas term = $-\frac{e\hbar}{4m^2c^2}\boldsymbol{\sigma}\cdot(\boldsymbol{E}\times\boldsymbol{p}) = -\frac{e\hbar}{4m^2c^2}(-\frac{1}{r}\frac{dV}{dr})\boldsymbol{\sigma}\cdot\boldsymbol{L} = \frac{e}{2m^2c^2}\frac{1}{r}\frac{dV}{dr}\boldsymbol{S}\cdot\boldsymbol{L}$

(Spin-orbit interaction)

The spin angular momentum is defined by

$$\boldsymbol{S} = \frac{\hbar}{2}\boldsymbol{\sigma}$$

which is an automatic consequence of the Dirac theory.

<u>The last term is called the Darwin term</u>.

For a hydrogen atom,

$$\nabla\cdot\mathbf{E} = -\delta^{(3)}(\mathbf{r}) .$$

It gives rise to an energy shift

$$\int\frac{e^2\hbar^2}{8m^2c^2}\delta^{(3)}(\mathbf{r})\left|\psi(\mathbf{r})^{(Schrodinger)}\right|^2 d^3x = \frac{e^2\hbar^2}{8m^2c^2}\left|\psi(\mathbf{r})^{(Schrodinger)}\right|^2_{\mathbf{r}=0}$$

which is non-vanishing only for the s state.

13. Free particle at rest

Each component of the four-component wave function satisfies the Klein-Gordon equation if the particle is free.

$$(\gamma_\mu\frac{\partial}{\partial x_\mu} + \frac{mc}{\hbar})\psi = 0 \tag{1}$$

$$\gamma_k = \begin{pmatrix} 0 & -i\sigma_k \\ i\sigma_k & 0 \end{pmatrix}$$

$$\gamma_4 = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}$$

Multiplying Eq.(1) from the left by $\gamma_\mu\frac{\partial}{\partial x_\mu}$

$$\gamma_\nu \frac{\partial}{\partial x_\nu}(\gamma_\mu \frac{\partial}{\partial x_\mu})\psi + \frac{mc}{\hbar}\gamma_\nu \frac{\partial}{\partial x_\nu}\psi = 0$$

$$\gamma_\nu \gamma_\mu \frac{\partial}{\partial x_\nu}\frac{\partial}{\partial x_\mu}\psi + \frac{mc}{\hbar}\gamma_\mu \frac{\partial}{\partial x_\mu}\psi = 0$$

$$\frac{1}{2}(\gamma_\nu\gamma_\mu + \gamma_\mu\gamma_\nu)\frac{\partial}{\partial x_\nu}\frac{\partial}{\partial x_\mu}\psi - (\frac{mc}{\hbar})^2\psi = 0$$

Since $\{\gamma_\mu, \gamma_\nu\} = 2\delta_{\mu,\nu}$, we have

$$\delta_{\mu,\nu}\frac{\partial}{\partial x_\nu}\frac{\partial}{\partial x_\mu}\psi - (\frac{mc}{\hbar})^2\psi = 0 \qquad (2)$$

Note that Eq.(2) is to be understood as four separate uncoupled equations for each component of ψ. Because of Eq.(2), the Dirac equation admits a free particle solution of the type

$$\psi \approx u(\mathbf{p})\exp[\frac{i}{\hbar}(\mathbf{p}\cdot\mathbf{r} - Et)]$$

with

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

$u(\boldsymbol{p})$ is a four-componenet spinor independent of $\boldsymbol{r}$ and t.

((Note)) The following relations are always valid.

$$i\hbar\frac{\partial}{\partial t}\psi = E\psi, \qquad \frac{\hbar}{i}\nabla\psi = \boldsymbol{p}\psi$$

For a particle at rest ($\boldsymbol{p} = 0$)

$$(\gamma_\mu \frac{\partial}{\partial x_\mu} + \frac{mc}{\hbar})\psi = 0$$

or

$$(\gamma_1 \frac{\partial}{\partial x_1} + \gamma_2 \frac{\partial}{\partial x_2} + \gamma_3 \frac{\partial}{\partial x_3} + \gamma_4 \frac{\partial}{\partial x_4} + \frac{mc}{\hbar})\psi = 0$$

Since

$$\frac{\hbar}{i}\nabla\psi = \boldsymbol{p}\psi = 0, \qquad E = \pm mc^2$$

$$[\gamma_4 \frac{\partial}{\partial(ict)} + \frac{mc}{\hbar}]\psi = 0$$

or

$$[\frac{1}{ic}\gamma_4 \frac{E}{i\hbar} + \frac{mc}{\hbar}]\psi = 0$$

or

$$\frac{E}{\hbar c}\gamma_4\psi = \frac{mc}{\hbar}\psi$$

For $E = mc^2$,

$$u = \begin{pmatrix} u_A(\mathbf{p}=0) \\ u_B(\mathbf{p}=0) \end{pmatrix}$$

$$\frac{mc^2}{\hbar c}\begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}\begin{pmatrix} u_A(\boldsymbol{p}=0) \\ u_B(\boldsymbol{p}=0) \end{pmatrix} = \frac{mc}{\hbar}\begin{pmatrix} u_A(\boldsymbol{p}=0) \\ u_B(\boldsymbol{p}=0) \end{pmatrix}$$

or

$$\begin{pmatrix} u_A(\boldsymbol{p}=0) \\ -u_B(\boldsymbol{p}=0) \end{pmatrix} = \begin{pmatrix} u_A(\boldsymbol{p}=0) \\ u_B(\boldsymbol{p}=0) \end{pmatrix}$$

or

$$u_B(\boldsymbol{p}=0)=0$$

For $E = -mc^2$,

$$u=\begin{pmatrix} u_A(\boldsymbol{p}=0) \\ u_B(\boldsymbol{p}=0) \end{pmatrix}$$

$$-\frac{mc^2}{\hbar c}\begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}\begin{pmatrix} u_A(\boldsymbol{p}=0) \\ u_B(\boldsymbol{p}=0) \end{pmatrix}=\frac{mc}{\hbar}\begin{pmatrix} u_A(\boldsymbol{p}=0) \\ u_B(\boldsymbol{p}=0) \end{pmatrix}$$

or

$$\begin{pmatrix} -u_A(\mathbf{p}=0) \\ u_B(\mathbf{p}=0) \end{pmatrix}=\begin{pmatrix} u_A(\mathbf{p}=0) \\ u_B(\mathbf{p}=0) \end{pmatrix}$$

$$u_A(\mathbf{p}=0)=0$$

So there are four independent solutions

Positive energy solution

$$\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}\exp(-i\frac{mc^2t}{\hbar}), \qquad \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}\exp(-i\frac{mc^2t}{\hbar}),$$

spin up spin down

Negative energy solution

$$\begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}\exp(i\frac{mc^2t}{\hbar}), \qquad \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}\exp(i\frac{mc^2t}{\hbar}),$$

The existence of negative-energy solutions is intimately related to the fact that the Dirac theory can accomodate a positron.

((Note))
Nonrelativistic limit $E = mc^2$, the upper two component spinor ψ_A coincides with the Schrödinger wave function apart from the factor $e^{-imc^2 t/\hbar}$.

Let us define

$$\Sigma_3 = \frac{\gamma_1\gamma_2 - \gamma_2\gamma_1}{2i} = \begin{pmatrix} \sigma_3 & 0 \\ 0 & \sigma_3 \end{pmatrix}$$

((Note))

$$\gamma_1\gamma_2 = \begin{pmatrix} 0 & -i\sigma_1 \\ i\sigma_1 & 0 \end{pmatrix}\begin{pmatrix} 0 & -i\sigma_2 \\ i\sigma_2 & 0 \end{pmatrix} = \begin{pmatrix} \sigma_1\sigma_2 & 0 \\ 0 & \sigma_1\sigma_2 \end{pmatrix}$$

Similarly

$$\gamma_2\gamma_1 = \begin{pmatrix} \sigma_2\sigma_1 & 0 \\ 0 & \sigma_2\sigma_1 \end{pmatrix}$$

$$\begin{aligned} \gamma_1\gamma_2 - \gamma_2\gamma_1 &= \begin{pmatrix} \sigma_1\sigma_2 - \sigma_2\sigma_1 & 0 \\ 0 & \sigma_1\sigma_2 - \sigma_2\sigma_1 \end{pmatrix} \\ &= 2\begin{pmatrix} \sigma_1\sigma_2 & 0 \\ 0 & \sigma_1\sigma_2 \end{pmatrix} \\ &= 2i\begin{pmatrix} \sigma_3 & 0 \\ 0 & \sigma_3 \end{pmatrix} \end{aligned}$$

$$\Sigma_3 \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} \sigma_3 & 0 \\ 0 & \sigma_3 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

The eigenstate of Σ_3 is interpreted as the spin component in the positive z-direction in units of $\hbar/2$.

---

14. Plane wave solutions ($p \neq 0$).

$$\psi = \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix} = \begin{pmatrix} u_A(\mathbf{p}) \\ u_B(\mathbf{p}) \end{pmatrix} \exp[\frac{i}{\hbar}(\mathbf{p}\cdot\mathbf{r} - Et)]$$

or

$$\frac{1}{c}(i\hbar\frac{\partial}{\partial t} - mc^2)\psi_A = (\boldsymbol{\sigma}\cdot\boldsymbol{p})\psi_B\,,$$

$$\frac{1}{c}(i\hbar\frac{\partial}{\partial t} + mc^2)\psi_B = (\boldsymbol{\sigma}\cdot\boldsymbol{p})\psi_A$$

or

$$(\boldsymbol{\sigma}\cdot\boldsymbol{p})u_B = \frac{1}{c}(E - mc^2)u_A\,, \qquad (\boldsymbol{\sigma}\cdot\boldsymbol{p})u_A = \frac{1}{c}(E + mc^2)u_B$$

or

$$u_A(\boldsymbol{p}) = \frac{c}{E - mc^2}(\boldsymbol{\sigma}\cdot\boldsymbol{p})u_B(\boldsymbol{p})$$

$$u_B(\boldsymbol{p}) = \frac{c}{E + mc^2}(\boldsymbol{\sigma}\cdot\boldsymbol{p})u_A(\boldsymbol{p})$$

Fro simplicity we use

$$R = \sqrt{\boldsymbol{p}^2c^2 + m^2c^4}$$

(i) For $E = R > 0$ (positive energy state)

$$u_A{}^{(1)}(\boldsymbol{p}) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad u_A{}^{(2)}(\boldsymbol{p}) = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$u_B^{(1)}(\boldsymbol{p}) = \frac{c}{R+mc^2}\begin{pmatrix} p_3 & p_1 - ip_2 \\ p_1 + ip_2 & -p_3 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$= \begin{pmatrix} \dfrac{cp_3}{R+mc^2} \\ \dfrac{c(p_1+ip_2)}{R+mc^2} \end{pmatrix}$$

$$u_B^{(2)}(\boldsymbol{p}) = \frac{c}{R+mc^2}\begin{pmatrix} p_3 & p_1 - ip_2 \\ p_1 + ip_2 & -p_3 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$= \begin{pmatrix} \dfrac{c(p_1-ip_2)}{R+mc^2} \\ -\dfrac{cp_3}{R+mc^2} \end{pmatrix}$$

Then we have

$$u^{(1)}(\boldsymbol{p}) = \sqrt{\frac{R+mc^2}{2R}}\begin{pmatrix} 1 \\ 0 \\ \dfrac{cp_3}{R+mc^2} \\ \dfrac{c(p_1+ip_2)}{R+mc^2} \end{pmatrix}, \qquad u^{(2)}(\boldsymbol{p}) = \sqrt{\frac{R+mc^2}{2R}}\begin{pmatrix} 0 \\ 1 \\ \dfrac{c(p_1-ip_2)}{R+mc^2} \\ -\dfrac{cp_3}{R+mc^2} \end{pmatrix}$$

We take into account of the normalization factor.

(ii) For $E = -R < 0$

$$u_B^{(1)}(\mathbf{p}) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad u_B^{(2)}(\mathbf{p}) = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$u_A^{(1)}(\boldsymbol{p}) = \frac{-c}{R+mc^2}\begin{pmatrix} p_3 & p_1 - ip_2 \\ p_1 + ip_2 & -p_3 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$= \begin{pmatrix} -\dfrac{cp_3}{R+mc^2} \\ -\dfrac{c(p_1+ip_2)}{R+mc^2} \end{pmatrix}$$

$$u_A^{(2)}(\boldsymbol{p}) = \frac{-c}{R+mc^2}\begin{pmatrix} p_3 & p_1 - ip_2 \\ p_1 + ip_2 & -p_3 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} -\dfrac{c(p_1 - ip_2)}{R+mc^2} \\ \dfrac{cp_3}{R+mc^2} \end{pmatrix}$$

Then we have

$$u^{(3)}(\boldsymbol{p}) = \sqrt{\frac{R+mc^2}{2R}}\begin{pmatrix} -\dfrac{cp_3}{R+mc^2} \\ -\dfrac{c(p_1+ip_2)}{R+mc^2} \\ 1 \\ 0 \end{pmatrix}, \qquad u^{(4)}(\boldsymbol{p}) = \sqrt{\frac{R+mc^2}{2R}}\begin{pmatrix} -\dfrac{c(p_1-ip_2)}{R+mc^2} \\ \dfrac{cp_3}{R+mc^2} \\ 0 \\ 1 \end{pmatrix}$$

---

15. Formulation

Since

$$u^{(r)}(\mathbf{p})\exp[\frac{i}{\hbar}\{\mathbf{p}\cdot\mathbf{r} - Et)]$$

satisfies the free-field Dirac equation

$$(\gamma_\mu \frac{\partial}{\partial x_\mu} + \frac{mc}{\hbar})\psi = 0,$$

$$\frac{\partial}{\partial x_k}\{u^{(r)}(\boldsymbol{p})\exp[\frac{i}{\hbar}\{\boldsymbol{p}\cdot\boldsymbol{r} - Et)]\} = u^{(r)}(\boldsymbol{p})\exp[\frac{i}{\hbar}\{\boldsymbol{p}\cdot\boldsymbol{r} - Et)]\frac{i}{\hbar}p_k$$

$$\begin{aligned}\frac{\partial}{\partial x_4}\{u^{(r)}(\boldsymbol{p})\exp[\frac{i}{\hbar}\{\boldsymbol{p}\cdot\boldsymbol{r} - Et)]\} &= u^{(r)}(\boldsymbol{p})\exp[\frac{i}{\hbar}\{\boldsymbol{p}\cdot\boldsymbol{r} - Et)](\frac{1}{ic})(-\frac{i}{\hbar}E) \\ &= u^{(r)}(\boldsymbol{p})\exp[\frac{i}{\hbar}\{\boldsymbol{p}\cdot\boldsymbol{r} - Et)](-\frac{E}{\hbar c})\end{aligned}$$

Since

$$p_\mu = (\mathbf{p}, i\frac{E}{c})$$

we get

$$\left(\frac{i}{\hbar} p_k \gamma_k - \frac{E}{\hbar c}\gamma_4 + \frac{mc}{\hbar}\right) u^{(r)}(p) = 0$$

or

$$\left(ip_k \gamma_k - \frac{E}{c}\gamma_4 + mc\right) u^{(r)}(p) = 0$$

or

$$(i\gamma \cdot p + mc) u^{(r)}(p) = 0$$

regardless of whether E>0 or E<0.

In summary we have

$$u^{(1)}(\boldsymbol{p}) = \sqrt{\frac{R+mc^2}{2R}} \begin{pmatrix} 1 \\ 0 \\ \dfrac{cp_3}{R+mc^2} \\ \dfrac{c(p_1+ip_2)}{R+mc^2} \end{pmatrix}, \qquad (E>0)$$

$$u^{(2)}(\boldsymbol{p}) = \sqrt{\frac{R+mc^2}{2R}} \begin{pmatrix} 0 \\ 1 \\ \dfrac{c(p_1-ip_2)}{R+mc^2} \\ -\dfrac{cp_3}{R+mc^2} \end{pmatrix}, \qquad (E>0)$$

$$u^{(3)}(\boldsymbol{p}) = \sqrt{\frac{R+mc^2}{2R}} \begin{pmatrix} -\dfrac{cp_3}{R+mc^2} \\ -\dfrac{c(p_1+ip_2)}{R+mc^2} \\ 1 \\ 0 \end{pmatrix}, \qquad (E<0)$$

$$u^{(4)}(\boldsymbol{p}) = \sqrt{\frac{R+mc^2}{2R}} \begin{pmatrix} -\frac{c(p_1 - ip_2)}{R+mc^2} \\ \frac{cp_3}{R+mc^2} \\ 0 \\ 1 \end{pmatrix}, \qquad (E<0)$$

Suppose that $\boldsymbol{p} = 0$. $R = mc^2$.

$$u^{(1)}(\boldsymbol{p}=0) = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \qquad u^{(2)}(\boldsymbol{p}=0) = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}.$$

$$u^{(3)}(\boldsymbol{p}=0) = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, u^{(4)}(\boldsymbol{p}=0) = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

The first two solutions look like the spin state of the non-relativistic theory. They are degenerate and have enery eigenvalue $E = R$. In the same limit, the last two solutions also look like the non-relativistic spin states, but they belong to the energy eigenvalue $E = -R$

---

13. Dirac's hole theory

13.1. Overview on Dirac's hole theory

Dirac made the astounding suggestion that all the negative-energy states should be already occupied. This ocean of occupied negative-energy states is now referred to as the ‘Dirac sea’. Thus, according to Dirac, the negative energy states are already full up; by the Pauli principle, there is now no room for an electron to fall into such a state. But, as Dirac further reasoned, occasionally there might be a few negative-energy states that are unoccupied. Such a ‘hole’ in the Dirac sea of negative-energy states would appear just like a positive-energy particle (and hence a positive-mass particle), whose electric charge would be the opposite of the charge on the electron. Such an empty negative-energy state could now be occupied by an ordinary electron; so the electron might ‘fall into’ that state with the emission of energy (normally in the form of electromagnetic radiation, i.e. photons). This would result in the ‘hole’ and the electron annihilating one another in the manner that we now understand as a particle and its anti-particle undergoing mutual annihilation.

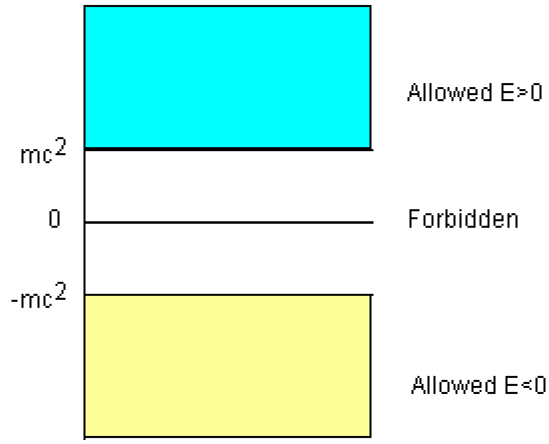


Fig. $2mc^2 = 1.02$ MeV.

Conversely, if a hole were not present initially, but a sufficient amount of energy (say in the form of photons) enters the system, then an electron can be kicked out of one of the negative-energy states to leave a hole. Dirac's 'hole' is indeed the electron's antiparticle, now referred to as the positron.

At first Dirac was cautious about making the claim that his theory actually predicted the existence of antiparticles to electrons, initially thinking (in 1929) that the 'holes' could be protons, which were the only massive particles known at the time having a positive charge. But it was not long before it became clear that the mass of each hole had to be equal to the mass of the electron, rather than the mass of a proton, which is about 1836 times larger. In the year 1931, Dirac came to the conclusion that the holes must be 'anti-electrons'—previously unknown particles that we now call positrons.

13.2 The discovery of positron by Carl D. Anderson

In the next year after Dirac's theoretical prediction, Carl Anderson announced the discovery of a particle which indeed had the properties that Dirac had predicted: the first antiparticle had been found!

Carl David Anderson (September 3, 1905 – January 11, 1991) was an American physicist. He is best known for his discovery of the positron in 1932, an achievement for which he received the 1936 Nobel Prize in Physics, and of the muon in 1936. Anderson was born in New York City, the son of Swedish immigrants. He studied physics and engineering at Caltech (B.S., 1927; Ph.D., 1930). Under the supervision of Robert A. Millikan, he began investigations into cosmic rays during the course of which he encountered unexpected particle tracks in his (modern versions now commonly referred to as an Anderson) cloud chamber photographs that he correctly interpreted as having been created by a particle with the same mass as the electron, but with opposite electrical charge. This discovery, announced in 1932 and later confirmed by others, validated Paul Dirac's theoretical prediction of the existence of the positron. Anderson first detected the particles in cosmic rays. He then produced more conclusive proof by shooting gamma rays produced by the natural radioactive nuclide ThC'' (^{208}Tl) into other materials, resulting in the creation of positron-electron pairs. For this work, Anderson shared the 1936 Nobel Prize in Physics with Victor Hess.

http://en.wikipedia.org/wiki/Carl_David_Anderson

13.2. Dirac sea

The Dirac equation for the free particle leads to a negative energy solution as well as a positive energy solution. The positive energy solutions and the negative solutions are separated by a gap shown in **Fig.1**. Classically, no transition is expected between the energy gap (= 2 mc^2). So we can restrict the energy to be positive classically. On the other hand, in quantum mechanics, it is expected that the transition can occur. Since electrons are fermions, all the negative-energy levels are filled with electrons, in accord with the Pauli exclusion principle. The vacuum state (so called Dirac sea) is one with all negative-energy levels filled and all positive-energy level empty. We note that the Dirac sea is a theoretical model of the vacuum as an infinite sea of particles with negative energy ($E<-mc^2$). The positron, the antimatter counterpart of the electron, was originally conceived of as a hole in the Dirac sea, well before its experimental discovery in 1932 (C.D. Anderson).

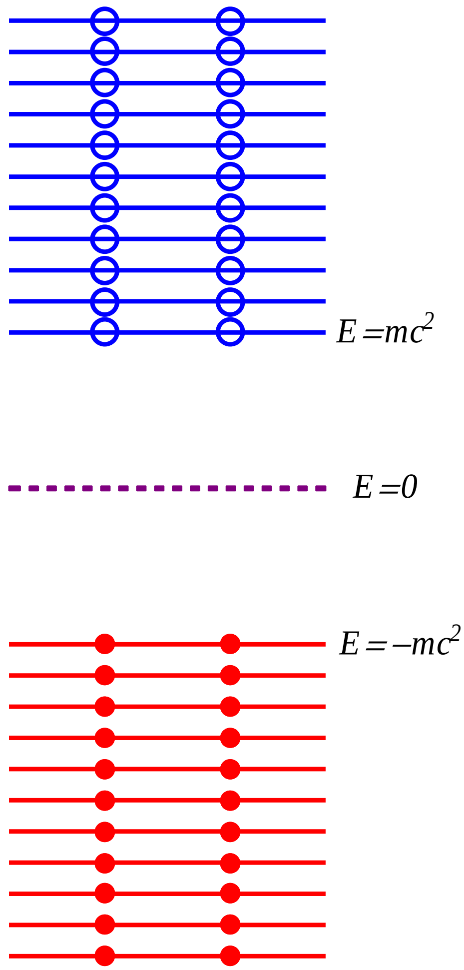


Fig.1 The Dirac sea. Positrons as holes in the Dirac sea of negative-energy electron states. Dirac proposed that almost all negative energy states of the electron are filled. Pauli principle prevents an electron from falling into such a filled state. The electron states with the energy above mc^2 (denoted by blue open circles) are empty.

<u>Charge:</u>

$$Q_{hole} = (Q_{vacuum} - (-|e|) - Q_{vacuum} = |e|$$

where Q_{vacuum} is infinite but we have seen such infinite renormalization before.

<u>Momentum:</u>

$$\boldsymbol{P}_{hole} = (\boldsymbol{P}_{vacuum} - \boldsymbol{p}) - \boldsymbol{P}_{vacuum} = -\boldsymbol{p}$$

where $\boldsymbol{P}_{vacuum} = 0$ since for each negative energy state with p there is another with (-$\boldsymbol{p}$)

Energy:

$$E_{hole} = [E_{vacuum} - (-R)] - E_{vacuum} = +R = \sqrt{m^2c^4 + c^2\boldsymbol{p}^2}$$

Spin:

$$\frac{\hbar}{2}\boldsymbol{\Sigma}_{hole} = (\frac{\hbar}{2}\boldsymbol{\Sigma}_{vacuum} - \frac{\hbar}{2}\boldsymbol{\Sigma}) - \frac{\hbar}{2}\boldsymbol{\Sigma}_{vacuum} = -\frac{\hbar}{2}\boldsymbol{\Sigma}$$

In summary

The positron is the antiparticle or the antimatter counterpart of the electron. The positron has an electric charge of +|*e*|, a spin of ½, and has the same mass as an electron.

Positive energy	$R = \sqrt{m^2c^4 + c^2\boldsymbol{p}^2}$
Positive charge	$\lvert e\rvert$ (>0)
Momentum	$-\boldsymbol{p}$
Spin	$-\frac{\hbar}{2}\boldsymbol{\Sigma}$
Helicity	$\boldsymbol{\Sigma}\cdot\hat{\boldsymbol{p}}$

13.3 Pair production

If sufficient energy (more than $2mc^2$) is given to the system in the form of radiation, one of the negative energy electrons is excited into an empty state with a positive energy. Thus we observe an electron of charge -|*e*| and energy *R*, and in addition a hole in the Dirac sea. This hole(anti-particle) has the same mass as the electron but opposite charge. This hole is called the positron. The process is called the pair production. The hole registers the absence of an electron of charge -|*e*| and energy –*R*, and would be interpreted by an observer relative to the vacuum as the presence a particle of charge |e| and energy *R*.

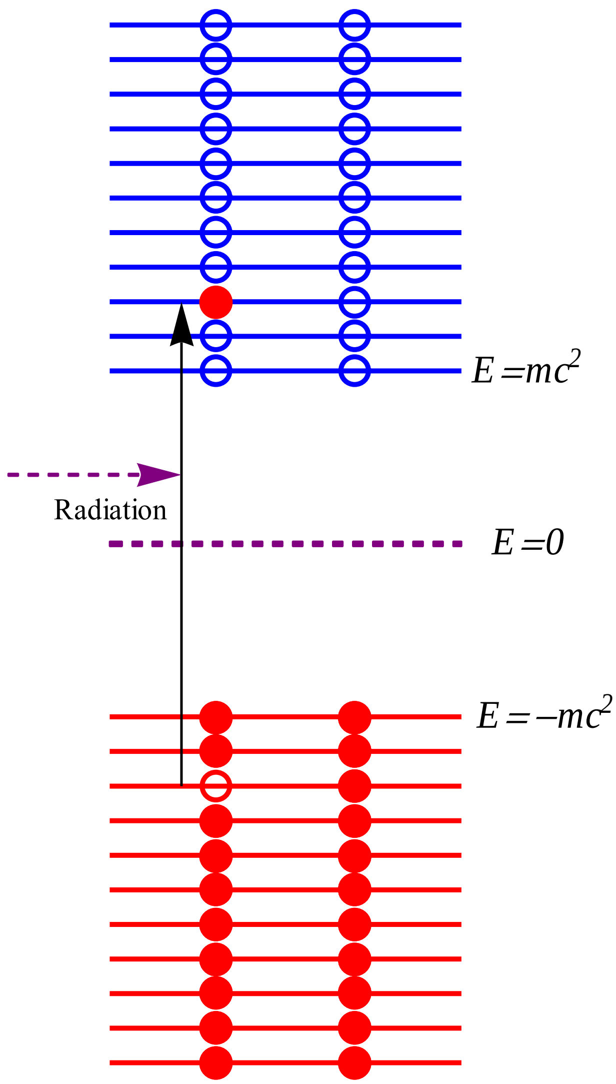


Fig.2 The pair production. The supplying of sufficient energy to the Dirac sea could produce an electron-positron pair: $\gamma \to e^{+} + e$.

13.4. Annihilation of electron and positron

When a low-energy positron collides with a low-energy electron, annihilation occurs, resulting in the production of gamma ray photons. An electron falling into a hole would be interpreted as the annihilation of the electron and the positron, with the release of energy in the form of radiation

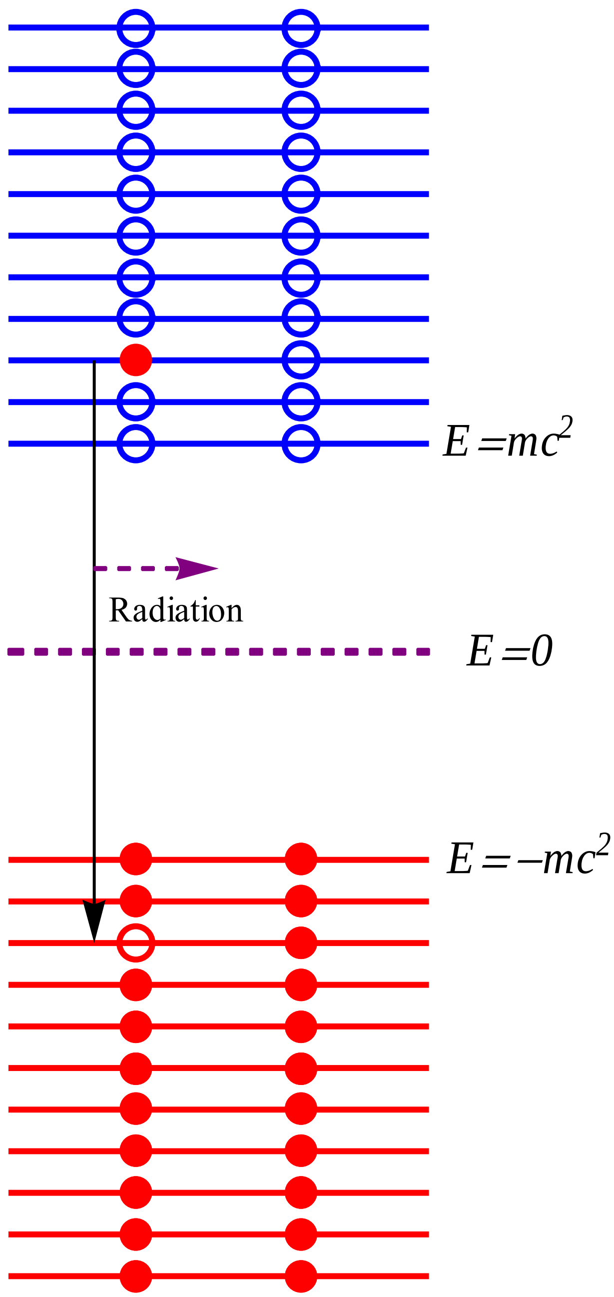


Fig.3 The annihilation of electron and positron; $e- + e+ \rightarrow \gamma + \gamma$

14. Orbital angular momentum *L*

The Hamiltonian of the free particle is given by

$$H = c\boldsymbol{\alpha}\cdot\boldsymbol{p} + \beta mc^2$$

The orbital angular momentum $\boldsymbol{L}$ is defined by

$$L_1 = x_2 p_3 - x_3 p_2, \qquad L_2 = x_3 p_1 - x_1 p_3, \qquad L_3 = x_1 p_2 - x_2 p_1$$

We now consider the commutation relation between these operators,

$$\begin{aligned}[H, L_1] &= [c\alpha_k p_k + \beta mc^2, x_2 p_3 - x_3 p_2] \\ &= [c\alpha_k p_k, x_2 p_3 - x_3 p_2] \\ &= [c\alpha_2 p_2, x_2 p_3] - [c\alpha_3 p_3, x_3 p_2] \\ &= c\alpha_2 [p_2, x_2] p_3 - c\alpha_3 [p_3, x_3] p_2 \\ &= \frac{c\hbar}{i}(\alpha_2 p_3 - \alpha_3 p_2) \\ &= \frac{c\hbar}{i}(\boldsymbol{\alpha} \times \boldsymbol{p})_1\end{aligned}$$

Then we get the Heisenberg's equation;

$$\frac{d\boldsymbol{L}}{dt} = \frac{i}{\hbar}[H, \boldsymbol{L}] = c(\boldsymbol{\alpha} \times \boldsymbol{p}).$$

15. Spin angular momentum $\frac{\hbar}{2}\boldsymbol{\Sigma}$

Here we note that

$$\Sigma_k = \begin{pmatrix} \sigma_k & 0 \\ 0 & \sigma_k \end{pmatrix} = -i\gamma_i\gamma_j \qquad (i, j, k;\ \text{cyclic})$$

or, simply,

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

$$\alpha_k = \begin{pmatrix} 0 & \sigma_k \\ \sigma_k & 0 \end{pmatrix} = i\gamma_4\gamma_k = -\Sigma_k\gamma_5 = -\gamma_5\Sigma_k$$

or, simply,

$$\boldsymbol{\alpha} = \begin{pmatrix} 0 & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & 0 \end{pmatrix}$$

with

$$[\gamma_5, \Sigma_k] = 0\,, \quad [\beta, \Sigma_k] = 0\,, \quad [\gamma_5, \alpha_k] = 0\,, \quad [\beta, \gamma_5] = 0$$

$$[\Sigma_i, \Sigma_j] = 2i\Sigma_k\,, \qquad \Sigma_i \Sigma_j = -\Sigma_j \Sigma_i = i\Sigma_k \qquad (i, j, \text{ and } k;\text{ cyclic})$$

$$[\gamma_5 \Sigma_k, \Sigma_j] = \gamma_5 \Sigma_k \Sigma_j - \Sigma_j \gamma_5 \Sigma_k = \gamma_5 [\Sigma_k, \Sigma_j]$$

((**Note**))

$$\Sigma_1 = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}, \qquad \Sigma_2 = \begin{pmatrix} 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \end{pmatrix}$$

$$\Sigma_3 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix},$$

$$\gamma_5 = \begin{pmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \\ -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}$$

Then we get

$$H = c\boldsymbol{\alpha} \cdot \boldsymbol{p} + \beta mc^2 = -c\gamma_5 \Sigma_k p_k + \beta mc^2$$

We consider the commutation relation,

$$
\begin{aligned}
[H, \Sigma_1] &= [-c\gamma_5 \Sigma_k p_k + \beta mc^2, \Sigma_1] \\
&= -cp_k[\gamma_5 \Sigma_k, \Sigma_1] + mc^2[\beta, \Sigma_1] \\
&= -cp_2[\gamma_5 \Sigma_2, \Sigma_1] - cp_3[\gamma_5 \Sigma_3, \Sigma_1] \\
&= cp_2 \gamma_5 [\Sigma_1, \Sigma_2] - cp_3 \gamma_5 [\Sigma_3, \Sigma_1] \\
&= 2icp_2 \gamma_5 \Sigma_3 - 2icp_3 \gamma_5 \Sigma_2 \\
&= 2ic(\alpha_2 p_3 - \alpha_3 p_2) \\
&= 2ic(\boldsymbol{\alpha} \times \boldsymbol{p})_1
\end{aligned}
$$

which leads to the Heisenberg's equation,

$$
\frac{d}{dt}\boldsymbol{\Sigma} = \frac{i}{\hbar}[H, \boldsymbol{\Sigma}] = \frac{i}{\hbar} 2ic(\boldsymbol{\alpha} \times \boldsymbol{p}) = -\frac{2c}{\hbar}(\boldsymbol{\alpha} \times \boldsymbol{p})
$$

16. Total angular momentum *J*

The time derivative of the total angular momentum ***J*** is obtained

$$
\frac{d}{dt}\boldsymbol{J} = \frac{d}{dt}(\boldsymbol{L} + \frac{\hbar}{2}\boldsymbol{\Sigma}) = c(\boldsymbol{\alpha} \times \boldsymbol{p}) - c(\boldsymbol{\alpha} \times \boldsymbol{p}) = 0
$$

Although $\boldsymbol{L}$ and $\frac{\hbar}{2}\boldsymbol{\Sigma}$ are not constants of the motion, the total angular momentum J should be identified with the total angular momentum and is a constant of the motion.

$$
\boldsymbol{J} = \boldsymbol{L} + \frac{\hbar}{2}\boldsymbol{\Sigma} = \begin{pmatrix} \boldsymbol{L} + \frac{\hbar}{2}\boldsymbol{\sigma} & 0 \\ 0 & \boldsymbol{L} + \frac{\hbar}{2}\boldsymbol{\sigma} \end{pmatrix}.
$$

As is well known, the constancy of ***J*** is a consequence of invariance under rotation. Hence ***J*** must be a constant of the motion even if a central (spherically symmetric) potential *V*(*r*) is added to the free particle Hamiltonian.

((**Note**))

$$
\langle \psi' | \hat{H} | \psi' \rangle = \langle \psi | \hat{H} | \psi \rangle
$$

or

$$\hat{R}_\alpha^{\ +}\hat{H}\hat{R}_\alpha = \hat{H}$$

with

$$|\psi'\rangle = \hat{R}_\alpha|\psi\rangle$$

Since

$$\hat{R}_\alpha = \exp(-\frac{i}{\hbar}\hat{J}_\alpha\theta)$$

$$[\hat{H},\hat{J}_\alpha] = 0 .$$

17. Helicity $\boldsymbol{\Sigma}\cdot\hat{\boldsymbol{p}}$

We define the helicity operator as

$$\boldsymbol{\Sigma}\cdot\hat{\boldsymbol{p}}$$

where $\hat{\boldsymbol{p}}$ is the unit vector ($\hat{\boldsymbol{p}} = \dfrac{\boldsymbol{p}}{p}$

$$\boldsymbol{\Sigma} = \begin{pmatrix} \boldsymbol{\sigma} & 0 \\ 0 & \boldsymbol{\sigma} \end{pmatrix}.$$

The eigenstate of helicity with eigenvalue +1 and -1 are referred to, respectively, as the right-handed state and the left-handed state.

$$\boldsymbol{\Sigma}\cdot\hat{\boldsymbol{p}} = \boldsymbol{\Sigma}\cdot\frac{\boldsymbol{p}}{p} = \frac{1}{p}\begin{pmatrix} \boldsymbol{\sigma}_1\cdot p_1 & 0 \\ 0 & \boldsymbol{\sigma}_1\cdot p_1 \end{pmatrix} + \frac{1}{p}\begin{pmatrix} \boldsymbol{\sigma}_2\cdot p_2 & 0 \\ 0 & \boldsymbol{\sigma}_2\cdot p_2 \end{pmatrix} + \frac{1}{p}\begin{pmatrix} \boldsymbol{\sigma}_3\cdot p_3 & 0 \\ 0 & \boldsymbol{\sigma}_3\cdot p_3 \end{pmatrix}$$

or

$$\boldsymbol{\Sigma}\cdot\hat{\boldsymbol{p}} = \frac{1}{p}\begin{pmatrix} p_3 & p_1 - ip_2 & 0 & 0 \\ p_1 + ip_2 & -p_3 & 0 & 0 \\ 0 & 0 & p_3 & p_1 - ip_2 \\ 0 & 0 & p_1 + ip_2 & -p_3 \end{pmatrix}$$

$$(\boldsymbol{\Sigma}\cdot\hat{\boldsymbol{p}})u^{(1)}(\boldsymbol{p}) = \frac{1}{p}\sqrt{\frac{R+mc^2}{2R}}\begin{pmatrix} p_3 & \frac{cp_3}{R+mc^2} & 0 & 0 \\ p_1+ip_2 & -p_3 & 0 & 0 \\ 0 & 0 & p_3 & p_1-ip_2 \\ 0 & 0 & p_1+ip_2 & -p_3 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \\ \frac{cp_3}{R+mc^2} \\ \frac{c(p_1+ip_2)}{R+mc^2} \end{pmatrix}$$

When $p_1 = p_2 = 0$ (for simplicity, p_3=1)

$$\boldsymbol{\Sigma}\cdot\hat{\boldsymbol{p}} = \Sigma_3$$

$$\Sigma_3 u^{(1)}(\boldsymbol{p}) = \sqrt{\frac{R+mc^2}{2R}}\begin{pmatrix} 1 & \frac{c}{R+mc^2} & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -\hat{p}_3 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \\ \frac{c}{R+mc^2} \\ 0 \end{pmatrix}$$

$$= \sqrt{\frac{R+mc^2}{2R}}\begin{pmatrix} 1 \\ 0 \\ \frac{cp_3}{R+mc^2} \\ 0 \end{pmatrix} = u^{(1)}(\boldsymbol{p})$$

where

$$R = \sqrt{\boldsymbol{p}^2c^2 + m^2c^4}$$

Similarly, we have

$$\Sigma_3 u^{(2)}(\boldsymbol{p}) = -u^{(2)}(\boldsymbol{p}),$$

$$\Sigma_3 u^{(3)}(\boldsymbol{p}) = u^{(3)}(\boldsymbol{p})$$

$$\Sigma_3 u^{(4)}(\boldsymbol{p}) = -u^{(4)}(\boldsymbol{p})$$

18. Plane wave solution

Hamiltonian

$$H = c\boldsymbol{\alpha}\cdot\hat{\boldsymbol{p}} + \beta mc^2$$

$$\alpha_k = \begin{pmatrix} 0 & \sigma_k \\ \sigma_k & 0 \end{pmatrix} = i\gamma_4\gamma_k = -\Sigma_k\gamma_5$$

$$\beta = \gamma_4 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\gamma_5 = \gamma_1\gamma_2\gamma_3\gamma_4 ,$$

$$\Sigma_k = -i\gamma_i\gamma_j \qquad (i, j, k; \text{ cyclic}).$$
$$\Sigma_1 = -i\gamma_2\gamma_3 ,$$
$$\Sigma_2 = -i\gamma_3\gamma_1 ,$$
$$\Sigma_3 = -i\gamma_1\gamma_2$$

$$\begin{aligned} H^2 &= [c\boldsymbol{\alpha}\cdot\hat{\boldsymbol{p}} + \beta mc^2][c\boldsymbol{\alpha}\cdot\hat{\boldsymbol{p}} + \beta mc^2] \\ &= c^2(\boldsymbol{\alpha}\cdot\hat{\boldsymbol{p}})^2 + \beta^2 m^2 c^4 + c(\boldsymbol{\alpha}\cdot\hat{\boldsymbol{p}})(\beta mc^2) + c(\beta mc^2)(\boldsymbol{\alpha}\cdot\hat{\boldsymbol{p}}) \end{aligned}$$

$$\begin{aligned} (\boldsymbol{\alpha}\cdot\hat{\boldsymbol{p}})(\boldsymbol{\alpha}\cdot\hat{\boldsymbol{p}}) &= (\alpha_i\cdot\hat{p}_i)(\alpha_j\cdot\hat{p}_j) \\ &= \alpha_i\alpha_j\hat{p}_i\hat{p}_j \\ &= \frac{1}{2}(\alpha_i\alpha_j + \alpha_j\alpha_i)\hat{p}_i\hat{p}_j \\ &= \frac{1}{2}2\delta_{ij}\hat{p}_i\hat{p}_j \\ &= \hat{\boldsymbol{p}}^2 \end{aligned}$$

Note that

$$\beta^2 = 1$$

$$(\boldsymbol{\alpha}\cdot\hat{\boldsymbol{p}})\beta + \beta(\boldsymbol{\alpha}\cdot\hat{\boldsymbol{p}}) = \alpha_i\hat{p}_i\beta + \beta\alpha_i\hat{p}_i = (\alpha_i\beta + \beta\alpha_i)\hat{p}_i = 0$$

Thus we have

$$H^2 = c^2\boldsymbol{p}^2 + m^2c^4 .$$

We now consider a plane wave given by

$$\psi = u(\mathbf{p})\exp[\frac{i}{\hbar}\{\mathbf{p}\cdot\mathbf{r} - Et)]$$

$$H = -ic\hbar\boldsymbol{\alpha}\cdot\nabla + \beta mc^2$$

$$H\psi = i\hbar\frac{\partial\psi}{\partial t}$$

Left-hand side

$$(-ic\hbar\boldsymbol{\alpha}\cdot\nabla + \beta mc^2)\psi = (-ic\hbar\boldsymbol{\alpha}\cdot\nabla + \beta mc^2)u(\boldsymbol{p})\exp[\frac{i}{\hbar}\{\boldsymbol{p}\cdot\boldsymbol{r} - Et)]$$
$$= (c\boldsymbol{\alpha}\cdot\boldsymbol{p} + \beta mc^2)\psi$$

right-hand side

$$i\hbar\frac{\partial\psi}{\partial t} = i\hbar u(\mathbf{p})(-\frac{i}{\hbar}E)\exp[\frac{i}{\hbar}\{\mathbf{p}\cdot\mathbf{r} - Et)] = E\psi$$

or

$$H\psi = E\psi$$

or

$$Hu(\mathbf{p}) = Eu(\mathbf{p})$$

where

$$H = c\boldsymbol{\alpha}\cdot\boldsymbol{p} + \beta mc^2$$

$$H^2u(\boldsymbol{p}) = EHu(\boldsymbol{p}) = E^2u(\boldsymbol{p})$$

or

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

or

$$E = \pm c\sqrt{\boldsymbol{p}^2 + m^2c^2}$$

We now discuss

$$Hu(\boldsymbol{p}) = Eu(\boldsymbol{p})$$

Since

$$H = c\boldsymbol{\alpha}\cdot\boldsymbol{p} + \beta mc^2 = c(i\gamma_4\gamma_k)p_k + \gamma_4 mc^2$$

$$[c(i\gamma_4\gamma_k)p_k + \gamma_4 mc^2]u(\boldsymbol{p}) = Eu(\boldsymbol{p})$$

Multiplying this equation by γ_4

$$(i\gamma_k p_k - \frac{E}{c}\gamma_4 + +mc)u(\mathbf{p}) = 0$$

Noting that

$$-\frac{E}{c}\gamma_4 = -p_0\gamma_4 = -\frac{1}{i}p_4\gamma_4 = ip_4\gamma_4\,, \qquad p_0 = E/c, \qquad p_4 = ip_0$$

we obtain

$$(i\gamma p + mc)u(\boldsymbol{p}) = 0$$

where $\gamma p = \gamma_\mu p_\mu$

19. Simultaneous eigenket of H and $\boldsymbol{\Sigma}\cdot\hat{\boldsymbol{p}}$.

We show that H is commutable with $\boldsymbol{\Sigma}\cdot\hat{\boldsymbol{p}}$.

$$\boldsymbol{\Sigma}\cdot\hat{\boldsymbol{p}} = \Sigma_k\hat{p}_k$$

$$\Sigma_k = \begin{pmatrix} \sigma_k & 0 \\ 0 & \sigma_k \end{pmatrix} = -i\gamma_i\gamma_j \qquad (i, j, k;\ \text{cyclic})$$

$$\alpha_k = \begin{pmatrix} 0 & \sigma_k \\ \sigma_k & 0 \end{pmatrix} = i\gamma_4\gamma_k = -\Sigma_k\gamma_5 = -\gamma_5\Sigma_k$$

where

$$[\gamma_5, \Sigma_k] = 0, \quad [\beta, \Sigma_k] = 0, \quad [\gamma_5, \alpha_k] = 0, \quad [\beta, \gamma_5] = 0$$

Suppose that $u(\boldsymbol{p})$ is the eigenket of H,

$$Hu(\boldsymbol{p}) = Eu(\boldsymbol{p})$$

with

$$H = c\boldsymbol{\alpha}\cdot\boldsymbol{p} + \beta mc^2 = -c\gamma_5\Sigma_k p_k + \beta mc^2$$

Here we note that

$$\begin{aligned}[H, \Sigma_j p_j] &= [-c\gamma_5\Sigma_k p_k + \beta mc^2, \Sigma_j p_j] \\ &= -cp_k p_j[\gamma_5\Sigma_k, \Sigma_j] + mc^2 p_j[\beta, \Sigma_j] \\ &= -cp_k p_j[\gamma_5\Sigma_k, \Sigma_j]\end{aligned}$$

We note that

$$[\gamma_5\Sigma_k, \Sigma_j] = \gamma_5\Sigma_k\Sigma_j - \Sigma_j\gamma_5\Sigma_k = \gamma_5[\Sigma_k, \Sigma_j]$$

$$[\Sigma_i, \Sigma_j] = 2i\Sigma_k, \qquad \Sigma_i\Sigma_j = -\Sigma_j\Sigma_i = i\Sigma_k \ \ (i, j, \text{ and } k;\ \text{cyclic})$$

Then

$$[H, \Sigma_j p_j] = -cp_k p_j\gamma_5[\Sigma_k, \Sigma_j] = -\frac{c}{2}p_k p_j\gamma_5[\Sigma_k, \Sigma_j] - \frac{c}{2}p_j p_k\gamma_5[\Sigma_j, \Sigma_k]$$

or

$$[H,\Sigma_j p_j] = -\frac{c}{2} p_k p_j \{\gamma_5[\Sigma_k,\Sigma_j] + \gamma_5[\Sigma_j,\Sigma_k]\} = 0$$

So we can demonstrate that

$$[H,\boldsymbol{\Sigma}\cdot\hat{\boldsymbol{p}}] = 0.$$

This implies that $u(\boldsymbol{p})$ is a simultaneous eigenket of H and $\boldsymbol{\Sigma}\cdot\hat{\boldsymbol{p}}$,

$$Hu(\boldsymbol{p}) = Eu(\boldsymbol{p}), \qquad (\boldsymbol{\Sigma}\cdot\hat{\boldsymbol{p}})u(\boldsymbol{p}) = hu(\boldsymbol{p})$$

with $\hat{\boldsymbol{p}} = \boldsymbol{p}/|\boldsymbol{p}|$. Since

$$\begin{aligned}
(\boldsymbol{\Sigma}\cdot\boldsymbol{p})(\boldsymbol{\Sigma}\cdot\boldsymbol{p}) &= (\Sigma_i p_i)(\Sigma_j p_j) \\
&= p_i p_j (\Sigma_i \Sigma_j) \\
&= \frac{1}{2} p_i p_j (\Sigma_i\Sigma_j + \Sigma_j\Sigma_i) \\
&= \boldsymbol{p}^2
\end{aligned}$$

or

$$(\boldsymbol{\Sigma}\cdot\boldsymbol{p})^2 = 1$$

$$(\boldsymbol{\Sigma}\cdot\boldsymbol{p})^2 u(\boldsymbol{p}) = h^2 u(\boldsymbol{p}) = u(\boldsymbol{p})$$

$$h^2 = 1, \qquad \text{or} \qquad h = \pm 1.$$

---

20. Classification of the simultaneous eigenket of *H* and the helicity

In summary, we have

$$Hu(\boldsymbol{p}) = Eu(\boldsymbol{p}), \qquad (\boldsymbol{\Sigma}\cdot\hat{\boldsymbol{p}})u(\boldsymbol{p}) = hu(\boldsymbol{p})$$

with $E = \pm c\sqrt{\boldsymbol{p}^2 + m^2c^2}$ and $h = \pm 1$.

$$\begin{pmatrix} E>0 \\ h=1 \end{pmatrix}, \qquad \begin{pmatrix} E>0 \\ h=-1 \end{pmatrix}, \qquad \begin{pmatrix} E<0 \\ h=1 \end{pmatrix}, \qquad \begin{pmatrix} E<0 \\ h=-1 \end{pmatrix}$$

Eigenket of the helicity

$$\boldsymbol{\Sigma}\cdot\hat{\boldsymbol{p}} = \begin{pmatrix} \boldsymbol{\sigma}\cdot\hat{\boldsymbol{p}} & 0 \\ 0 & \boldsymbol{\sigma}\cdot\hat{\boldsymbol{p}} \end{pmatrix}, \qquad u = \begin{pmatrix} u_A \\ u_B \end{pmatrix}$$

$$(\boldsymbol{\Sigma}\cdot\hat{\boldsymbol{p}})u = \begin{pmatrix} \boldsymbol{\sigma}\cdot\hat{\boldsymbol{p}} & 0 \\ 0 & \boldsymbol{\sigma}\cdot\hat{\boldsymbol{p}} \end{pmatrix}\begin{pmatrix} u_A \\ u_B \end{pmatrix} = h\begin{pmatrix} u_A \\ u_B \end{pmatrix}$$

or

$$\begin{pmatrix} (\boldsymbol{\sigma}\cdot\hat{\boldsymbol{p}})u_A \\ (\boldsymbol{\sigma}\cdot\hat{\boldsymbol{p}})u_B \end{pmatrix} = h\begin{pmatrix} u_A \\ u_B \end{pmatrix}$$

or

$$(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{p}})u_A = hu_A, \qquad (\boldsymbol{\sigma}\cdot\hat{\boldsymbol{p}})u_B = hu_B \qquad (1)$$

with $h = \pm 1$.

Eigenvalue problem with the Hamiltonian

$$\begin{aligned} H &= c\boldsymbol{\alpha}\cdot\boldsymbol{p} + \beta mc^2 \\ &= c\begin{pmatrix} 0 & \boldsymbol{\sigma}\cdot\boldsymbol{p} \\ \boldsymbol{\sigma}\cdot\boldsymbol{p} & 0 \end{pmatrix} + mc^2\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \\ &= \begin{pmatrix} mc^2 & c(\boldsymbol{\sigma}\cdot\boldsymbol{p}) \\ c(\boldsymbol{\sigma}\cdot\boldsymbol{p}) & -mc^2 \end{pmatrix} \end{aligned}$$

Eigenvalue problem:

$$Hu(\boldsymbol{p}) = Eu(\boldsymbol{p})$$

or

$$\begin{pmatrix} mc^2 & c(\boldsymbol{\sigma}\cdot\boldsymbol{p}) \\ c(\boldsymbol{\sigma}\cdot\boldsymbol{p}) & -mc^2 \end{pmatrix}\begin{pmatrix} u_A \\ u_B \end{pmatrix} = E\begin{pmatrix} u_A \\ u_B \end{pmatrix}$$

$$mc^2 u_A + c(\boldsymbol{\sigma}\cdot\boldsymbol{p})u_B = Eu_A$$

$$c(\boldsymbol{\sigma}\cdot\boldsymbol{p})u_A - mc^2 u_B = Eu_B$$

or

$$u_A = \frac{c(\boldsymbol{\sigma}\cdot\boldsymbol{p})u_B}{E - mc^2} = \frac{cp}{E - mc^2}(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{p}})u_B \tag{2}$$

$$u_B = \frac{c(\boldsymbol{\sigma}\cdot\boldsymbol{p})u_A}{E + mc^2} = \frac{cp}{E + mc^2}(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{p}})u_A$$

(i) $h = 1$ and $E>0$

$$(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{p}})u_A = u_A, \qquad (\boldsymbol{\sigma}\cdot\hat{\boldsymbol{p}})u_B = u_B$$

$$u_A = \frac{cp}{R - mc^2}(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{p}})u_B = \frac{cp}{R - mc^2}u_B$$

$$u_B = \frac{cp}{R + mc^2}(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{p}})u_A = \frac{cp}{R + mc^2}u_A$$

We choose

$$u_A = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad u_B = \begin{pmatrix} \dfrac{cp}{R + mc^2} \\ 0 \end{pmatrix}$$

or

$$u^{(1)} = \begin{pmatrix} 1 \\ 0 \\ \dfrac{cp}{R + mc^2} \\ 0 \end{pmatrix}$$

(ii) $h = -1$ and $E>0$

$$(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{p}})u_A = -u_A, \qquad (\boldsymbol{\sigma}\cdot\hat{\boldsymbol{p}})u_B = -u_B$$

$$u_A = \frac{cp}{E - mc^2}(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{p}})u_B = -\frac{cp}{R - mc^2}u_B$$

$$u_B = \frac{cp}{E + mc^2}(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{p}})u_A = -\frac{cp}{R + mc^2}u_A$$

We choose

$$u_A = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \qquad u_B = \begin{pmatrix} 0 \\ -\dfrac{cp}{R + mc^2} \end{pmatrix}$$

or

$$u^{(2)} = \begin{pmatrix} 0 \\ 1 \\ -\dfrac{cp}{R + mc^2} \\ 0 \end{pmatrix}$$

(iii) $h = 1$ and $E<0$

$$(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{p}})u_B = u_B, \qquad (\boldsymbol{\sigma}\cdot\hat{\boldsymbol{p}})u_A = u_A$$

$$u_A = -\frac{cp}{R + mc^2}(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{p}})u_B = -\frac{cp}{R + mc^2}u_B$$

$$u_B = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad u_A = \begin{pmatrix} -\dfrac{cp}{R + mc^2} \\ 0 \end{pmatrix}$$

or

$$u^{(3)} = \begin{pmatrix} -\dfrac{cp}{R+mc^2} \\ 0 \\ 1 \\ 0 \end{pmatrix}$$

(iv) h = -1 and E<0

$$(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{p}})u_B = -u_B$$

$$u_A = -\frac{cp}{R+mc^2}(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{p}})u_B = \frac{cp}{R+mc^2}u_B$$

$$u_B = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \qquad u_A = \begin{pmatrix} 0 \\ \dfrac{cp}{R+mc^2} \end{pmatrix}$$

or

$$u^{(4)} = \begin{pmatrix} 0 \\ \dfrac{cp}{R+mc^2} \\ 0 \\ 1 \end{pmatrix}$$

21. Foldy-Wouthuysen (FW) transformation

Discussion

$$H|a_n\rangle = E_n|a_n\rangle \qquad\qquad H|\psi\rangle = E_n|\psi\rangle$$

$$|\psi\rangle = |a_n\rangle,$$

Suppose that

$$U|b_n\rangle = |a_n\rangle \qquad\qquad U|\psi'\rangle = |\psi\rangle$$

$$|\psi'\rangle = |b_n\rangle$$

Then we have

$$HU|b_n\rangle = E_n U|b_n\rangle \qquad HU|\psi'\rangle = E_n U|\psi'\rangle$$

or

$$U^+HU|b_n\rangle = E_a|b_n\rangle \qquad U^+HU|\psi'\rangle = E_n|\psi'\rangle$$

Here we define

$$H' = U^+HU$$

Then we get

$$H'|b_n\rangle = E_n|b_n\rangle \qquad H'|\psi'\rangle = E_n|\psi'\rangle$$

Then $|\psi'\rangle$ is the eigenket of *H'* with the same eigenvalue E_n.

Suppose that

$$U = e^{-iS}$$

with *S* is the Hermitian operator. Then we have

$$H' = e^{iS}He^{iS}$$

We note that

$$\langle\psi|H|\psi\rangle = \langle\psi'|H'|\psi'\rangle \qquad \text{(from the definition)}$$

since

$$U|\psi'\rangle = |\psi\rangle, \qquad \langle\psi| = \langle\psi'|U^+$$

Then we have

$$\langle\psi|H|\psi\rangle = \langle\psi'|U^+HU|\psi'\rangle = \langle\psi'|H'|\psi'\rangle$$

or

$$H' = U^+HU$$

$$U = e^{-iS}$$

$$|\psi'\rangle = U^{+}|\psi\rangle = e^{iS}|\psi\rangle \qquad\qquad |\psi\rangle = U|\psi'\rangle = e^{-iS}|\psi'\rangle$$

$$H' = U^{+}HU = e^{iS}He^{-iS}$$

We choose S of the form

$$S = -\frac{i}{p}\beta(\boldsymbol{\alpha}\cdot\boldsymbol{p})\theta\,, \qquad\qquad e^{iS} = \exp[\frac{1}{p}\beta(\boldsymbol{\alpha}\cdot\boldsymbol{p})\theta]$$

θ is a real function to be determined. S is a Hermitian operator.

$$S^{+} = \frac{i}{p}(\boldsymbol{\alpha}^{+}\cdot\boldsymbol{p})\beta^{+}\theta(\boldsymbol{p}) = \frac{i}{p}(\boldsymbol{\alpha}\cdot\boldsymbol{p})\beta\theta(\boldsymbol{p}) = -\frac{i}{p}\beta(\boldsymbol{\alpha}\cdot\boldsymbol{p})\theta(\boldsymbol{p})$$

since $\{\alpha_i, \beta\} = 0$.

$$\begin{aligned} H' &= e^{iS}He^{-iS} \\ &= e^{iS}(c\boldsymbol{\alpha}\cdot\boldsymbol{p} + \beta mc^2)e^{-iS} \\ &= e^{iS}[\beta(c\beta\boldsymbol{\alpha}\cdot\boldsymbol{p}) + \beta mc^2)e^{-iS} \\ &= e^{iS}\beta(c\beta\boldsymbol{\alpha}\cdot\boldsymbol{p} + mc^2)e^{-iS} \\ &= e^{iS}\beta e^{-iS}e^{iS}(c\beta\boldsymbol{\alpha}\cdot\boldsymbol{p} + mc^2)e^{-iS} \\ &= e^{iS}\beta e^{-iS}(c\beta\boldsymbol{\alpha}\cdot\boldsymbol{p} + mc^2) \end{aligned}$$

since $[S, \beta\boldsymbol{\alpha}\cdot\boldsymbol{p}] = 0$. Furthermore

$$\beta e^{-iS} = e^{iS}\beta$$

So that

$$H' = e^{2iS}\beta(c\beta\boldsymbol{\alpha}\cdot\boldsymbol{p} + mc^2) = e^{2iS}(c\boldsymbol{\alpha}\cdot\boldsymbol{p} + \beta mc^2)$$

where $\beta^2 = 1$

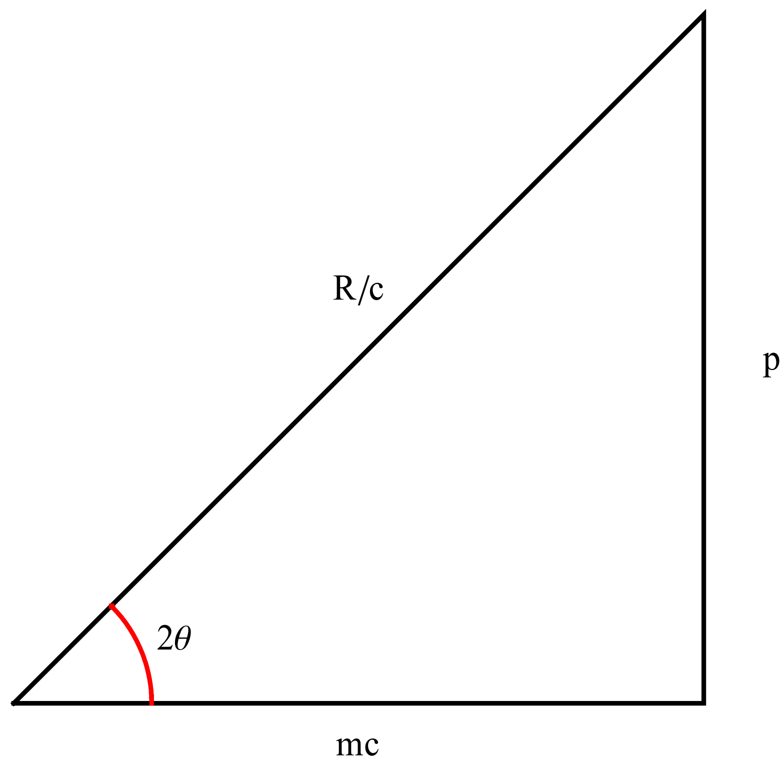
$$\begin{aligned} H' &= (\cos 2\theta + \frac{\beta\boldsymbol{\alpha}\cdot\boldsymbol{p}}{p}\sin 2\theta)(c\boldsymbol{\alpha}\cdot\boldsymbol{p} + \beta mc^2) \\ &= \beta(mc^2\cos 2\theta + cp\sin 2\theta) + \frac{\boldsymbol{\alpha}\cdot\boldsymbol{p}}{p}(pc\cos 2\theta - mc^2\sin 2\theta) \end{aligned}$$

where

$$(\boldsymbol{\alpha}\cdot\boldsymbol{p})(\boldsymbol{\alpha}\cdot\boldsymbol{p}) = p^2$$

and

$$e^{2iS} = \cos 2\theta + \frac{\beta\boldsymbol{\alpha}\cdot\boldsymbol{p}}{p}\sin 2\theta \qquad \text{(see the Mathematica)}$$



If we choose (so that odd terms disappear)

$$\tan 2\theta = \frac{p}{mc}.$$

$$\sin 2\theta = \frac{p}{\sqrt{p^2 + m^2c^2}} = \frac{cp}{R}, \qquad \cos 2\theta = \frac{mc}{\sqrt{p^2 + m^2c^2}} = \frac{mc^2}{R}$$

Then we have

$$
\begin{aligned}
H' &= \beta(mc^2\cos 2\theta + cp\sin 2\theta) \\
&= \beta(mc^2\frac{mc}{\sqrt{p^2+m^2c^2}} + cp\frac{p}{\sqrt{p^2+m^2c^2}}) \\
&= \beta c(\frac{m^2c^2}{\sqrt{p^2+m^2c^2}} + \frac{p^2}{\sqrt{p^2+m^2c^2}}) \\
&= \beta c\sqrt{p^2+m^2c^2} = \beta R
\end{aligned}
$$

where

$$
R = c\sqrt{p^2+m^2c^2}
$$

So that, H' is now diagonalized. The eigenstate of H' is the same as that of β.

$$
\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \qquad \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \qquad \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} \qquad \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}
$$

$$
|\psi\rangle = U|\psi'\rangle = e^{-iS}|\psi'\rangle
$$

where

$$
e^{-iS} = \begin{pmatrix}
\cos\theta & 0 & -\frac{p_z}{p}\sin\theta & -\frac{(p_x - ip_y)}{p}\sin\theta \\
0 & \cos\theta & -\frac{(p_x + ip_y)}{p}\sin\theta & \frac{p_z}{p}\sin\theta \\
\frac{p_z}{p}\sin\theta & \frac{(p_x - ip_y)}{p}\sin\theta & \cos\theta & 0 \\
\frac{(p_x + ip_y)}{p}\sin\theta & -\frac{p_z}{p}\sin\theta & 0 & \cos\theta
\end{pmatrix}
$$

Note that

$$
\cos\theta = \sqrt{\frac{1}{2}(1+\cos 2\theta)} = \sqrt{\frac{R+mc^2}{2R}}
$$

$$
\sin\theta = \sqrt{\frac{1}{2}(1-\cos 2\theta)} = \sqrt{\frac{R-mc^2}{2R}}
$$

Then the eigenstate of the original Hamiltonian H is given by

$$\begin{pmatrix} \cos\theta \\ 0 \\ \frac{p_z}{p}\sin\theta \\ \frac{(p_x+ip_y)}{p}\sin\theta \end{pmatrix} = \sqrt{\frac{R+mc^2}{2R}} \begin{pmatrix} 1 \\ 0 \\ \frac{cp_z}{R+mc^2} \\ \frac{c(p_x+ip_y)}{R+mc^2} \end{pmatrix}$$

$$\begin{pmatrix} 0 \\ \cos\theta \\ \frac{(p_x-ip_y)}{p}\sin\theta \\ -\frac{p_z}{p}\sin\theta \end{pmatrix} = \sqrt{\frac{R+mc^2}{2R}} \begin{pmatrix} 0 \\ 1 \\ \frac{c(p_x-ip_y)}{R+mc^2} \\ -\frac{cp_z}{R+mc^2} \end{pmatrix}$$

$$\begin{pmatrix} -\frac{p_z}{p}\sin\theta \\ -\frac{(p_x+ip_y)}{p}\sin\theta \\ \cos\theta \\ 0 \end{pmatrix} = \sqrt{\frac{R+mc^2}{2R}} \begin{pmatrix} -\frac{cp_z}{R+mc^2} \\ \frac{c(p_x+ip_y)}{R+mc^2} \\ 1 \\ 0 \end{pmatrix}$$

$$\begin{pmatrix} -\frac{(p_x-ip_y)}{p}\sin\theta \\ \frac{p_z}{p}\sin\theta \\ 0 \\ \cos\theta \end{pmatrix} = \sqrt{\frac{R+mc^2}{2R}} \begin{pmatrix} -\frac{c(p_x-ip_y)}{R+mc^2} \\ \frac{cp_z}{R+mc^2} \\ 0 \\ 1 \end{pmatrix}$$

((**Mathematica**))

```
Clear["Global`*"]; σx = (0 1
                          1 0); σy = (0 -ⅈ
                                      ⅈ  0); σz = (1  0
                                                   0 -1);
I2 = IdentityMatrix[2]; I4 = IdentityMatrix[4];
αx = KroneckerProduct[σx, σx]; αy = KroneckerProduct[σx, σy];
αz = KroneckerProduct[σx, σz];
β = KroneckerProduct[σz, I2];

H1 = c px αx + c py αy + c pz αz + β m^2 c^2 // Simplify;
S = -ⅈ (1/p) β.(αx px + αy py + αz pz) θ;

K1 =
  MatrixExp[2 ⅈ S] //. {Sqrt[-px^2 - py^2 - pz^2] → ⅈ p,
      1/(px^2 + py^2 + pz^2) → 1/p^2} // ExpToTrig // Simplify;

K11 = K1 /. {px^2 + py^2 + pz^2 → p^2} // Simplify;
K2 = (Cos[2 θ] I4 + (1/p) β.(αx px + αy py + αz pz) Sin[2 θ]) // Simplify;
K2 // MatrixForm
```

$$\begin{pmatrix} \text{Cos}[2\,\theta] & 0 & \frac{\text{pz Sin}[2\,\theta]}{\text{p}} & \frac{(\text{px}-\text{i py})\,\text{Sin}[2\,\theta]}{\text{p}} \\ 0 & \text{Cos}[2\,\theta] & \frac{(\text{px}+\text{i py})\,\text{Sin}[2\,\theta]}{\text{p}} & -\frac{\text{pz Sin}[2\,\theta]}{\text{p}} \\ -\frac{\text{pz Sin}[2\,\theta]}{\text{p}} & -\frac{(\text{px}-\text{i py})\,\text{Sin}[2\,\theta]}{\text{p}} & \text{Cos}[2\,\theta] & 0 \\ -\frac{(\text{px}+\text{i py})\,\text{Sin}[2\,\theta]}{\text{p}} & \frac{\text{pz Sin}[2\,\theta]}{\text{p}} & 0 & \text{Cos}[2\,\theta] \end{pmatrix}$$

```
K11 - K2 // Simplify

{{0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}}

Eigensystem[β]

{{-1, -1, 1, 1}, {{0, 0, 0, 1}, {0, 0, 1, 0}, {0, 1, 0, 0}, {1, 0, 0, 0}}}

MatrixExp[ⅈ S].β.MatrixExp[ⅈ S] - β // Simplify

{{0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}}
```

```
K3 =
  MatrixExp[ - i S] //. {Sqrt[-px^2 - py^2 - pz^2] → i p,
      1/(px^2 + py^2 + pz^2) → 1/p^2} // ExpToTrig // Simplify;

K31 = K3 /. {px^2 + py^2 + pz^2 → p^2} // Simplify;

K31 // MatrixForm
```

$$\begin{pmatrix} \text{Cos}[\theta] & 0 & -\frac{\text{pz Sin}[\theta]}{\text{p}} & -\frac{(\text{px}-i\,\text{py})\,\text{Sin}[\theta]}{\text{p}} \\ 0 & \text{Cos}[\theta] & -\frac{(\text{px}+i\,\text{py})\,\text{Sin}[\theta]}{\text{p}} & \frac{\text{pz Sin}[\theta]}{\text{p}} \\ \frac{\text{pz Sin}[\theta]}{\text{p}} & \frac{(\text{px}-i\,\text{py})\,\text{Sin}[\theta]}{\text{p}} & \text{Cos}[\theta] & 0 \\ \frac{(\text{px}+i\,\text{py})\,\text{Sin}[\theta]}{\text{p}} & -\frac{\text{pz Sin}[\theta]}{\text{p}} & 0 & \text{Cos}[\theta] \end{pmatrix}$$

22. Charge conjugate operator

We start with the Dirac equation for the free particle.
Dirac equation:

$$(\gamma_\mu \frac{\partial}{\partial x_\mu} + \frac{mc}{\hbar})\psi = 0$$

The replacement of

$$\frac{\partial}{\partial x_\mu} \to \frac{\partial}{\partial x_\mu} - \frac{ie}{\hbar c}A_\mu$$

leads to the Dirac equation in the presence of $A_\mu = (\boldsymbol{A}, iA_0)$

$$\gamma_\mu (\frac{\partial}{\partial x_\mu} - \frac{ie}{\hbar c}A_\mu)\psi + \frac{mc}{\hbar}\psi = 0$$

or

$$(\frac{\partial}{\partial x_\mu} - \frac{ie}{\hbar c}A_\mu)\gamma_\mu \psi + \frac{mc}{\hbar}\psi = 0 \qquad (1)$$

Hermite conjugate of Eq.(1):

$$(\frac{\partial}{\partial x_k} + \frac{ie}{\hbar c}A_k)\psi^+ \gamma_k + (\frac{\partial}{\partial x_4^*} + \frac{ie}{\hbar c}A_4^*)\psi^+ \gamma_4 + \frac{mc}{\hbar}\psi^+ = 0$$

or

$$(\frac{\partial}{\partial x_k}+\frac{ie}{\hbar c}A_k)\psi^+\gamma_k-(\frac{\partial}{\partial x_4}+\frac{ie}{\hbar c}A_4)\psi^+\gamma_4+\frac{mc}{\hbar}\psi^+=0$$

Multiplying Eq.(1) by γ_4 from the right, we get

$$(\frac{\partial}{\partial x_k}+\frac{ie}{\hbar c}A_k)\psi^+\gamma_k\gamma_4-(\frac{\partial}{\partial x_4}+\frac{ie}{\hbar c}A_4)\psi^+\gamma_4{}^2+\frac{mc}{\hbar}\psi^+\gamma_4=0$$

Here we note that

$$\psi^+\gamma_4=\overline{\psi}\,,\qquad\qquad \{\gamma_k,\gamma_4\}=0\,,$$

Then we get

$$-(\frac{\partial}{\partial x_k}+\frac{ie}{\hbar c}A_k)\psi^+\gamma_4\gamma_k-(\frac{\partial}{\partial x_4}+\frac{ie}{\hbar c}A_4)\psi^+\gamma_4\gamma_4+\frac{mc}{\hbar}\psi^+\gamma_4=0$$

or

$$-(\frac{\partial}{\partial x_k}+\frac{ie}{\hbar c}A_k)\overline{\psi}\gamma_k-(\frac{\partial}{\partial x_4}+\frac{ie}{\hbar c}A_4)\overline{\psi}\gamma_4+\frac{mc}{\hbar}\overline{\psi}=0$$

or

$$-(\frac{\partial}{\partial x_\mu}+\frac{ie}{\hbar c}A_\mu)\overline{\psi}\gamma_\mu+\frac{mc}{\hbar}\overline{\psi}=0 \qquad (2)$$

We consider the Dirac equation for the charge conjugate wave function ψ^C,

$$(\frac{\partial}{\partial x_\mu}+\frac{ie}{\hbar c}A_\mu)\gamma_\mu\psi^C+\frac{mc}{\hbar}\psi^C=0 \qquad (3)$$

We assume that

$$\psi^C=C\overline{\psi}^T$$

Then we get

$$(\frac{\partial}{\partial x_\mu}+\frac{ie}{\hbar c}A_\mu)\gamma_\mu C\overline{\psi}^T+\frac{mc}{\hbar}C\overline{\psi}^T=0 \tag{4}$$

Taking the transpose of Eq.(4), we get

$$(\frac{\partial}{\partial x_\mu}+\frac{ie}{\hbar c}A_\mu)\overline{\psi}C^T\gamma_\mu{}^T+\frac{mc}{\hbar}\overline{\psi}C^T=0\,. \tag{5}$$

Multiplying Eq.(5) by $(C^T)^{-1}$ from the right,

$$(\frac{\partial}{\partial x_\mu}+\frac{ie}{\hbar c}A_\mu)\overline{\psi}C^T\gamma_\mu{}^T(C^T)^{-1}+\frac{mc}{\hbar}\overline{\psi}=0\,, \tag{6}$$

Comparing Eq.(6) with Eq.(2), we havbe

$$C^T\gamma_\mu{}^T(C^T)^{-1}=-\gamma_\mu$$

or

$$C^{-1}\gamma_\mu C=-\gamma_\mu{}^T$$

Note that

$$\gamma_1{}^T=-\gamma_1\,,\qquad \gamma_2{}^T=\gamma_2\,,\qquad \gamma_3{}^T=-\gamma_3\,,\qquad \gamma_4{}^T=\gamma_4$$

Then we have

$$[\gamma_1,C]=0\,,\qquad [\gamma_3,C]=0$$

$$\{\gamma_2,C\}=0\,,\qquad \{\gamma_4,C\}=0$$

The above relations can be satisfied when

$$C=\gamma_2\gamma_4=\begin{pmatrix}0&0&0&1\\0&0&-1&0\\0&1&0&0\\-1&0&0&0\end{pmatrix}.$$

$$C^T=(\gamma_2\gamma_4)^T=\gamma_4{}^T\gamma_2{}^T=\gamma_4\gamma_2=-\gamma_2\gamma_4=-C$$

(see the Mathematica program below)

Then we have

$$\psi^C = C\overline{\psi}^T = \gamma_2\gamma_4(\psi^+\gamma_4)^T = \gamma_2\gamma_4\gamma_4{}^T(\psi^+)^T = \gamma_2\gamma_4\gamma_4\psi^* = \gamma_2\psi^*$$

where

$$\gamma_2 = -i\beta\alpha_2 = \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}$$

((**Example**))

$$\gamma_2 u_1{}^* = \sqrt{\frac{R+mc^2}{2R}} \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ \dfrac{cp_z}{R+mc^2} \\ \dfrac{c(p_x+ip_y)}{R+mc^2} \end{pmatrix} = \sqrt{\frac{R+mc^2}{2R}} \begin{pmatrix} -\dfrac{c(p_1+ip_2)}{R+mc^2} \\ \dfrac{cp_3}{R+mc^2} \\ 0 \\ -1 \end{pmatrix}$$

$$\gamma_2 u_2{}^* = \sqrt{\frac{R+mc^2}{2R}} \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ \dfrac{c(p_x-ip_y)}{R+mc^2} \\ -\dfrac{cp_z}{R+mc^2} \end{pmatrix} = \sqrt{\frac{R+mc^2}{2R}} \begin{pmatrix} \dfrac{cp_3}{R+mc^2} \\ \dfrac{c(p_1+ip_2)}{R+mc^2} \\ 1 \\ 0 \end{pmatrix}$$

$$\gamma_2 u_3{}^* = \sqrt{\frac{R+mc^2}{2R}} \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \dfrac{-cp_3}{R+mc^2} \\ \dfrac{-c(p_1-ip_2)}{R+mc^2} \\ 1 \\ 0 \end{pmatrix} = \sqrt{\frac{R+mc^2}{2R}} \begin{pmatrix} 0 \\ 1 \\ -\dfrac{c(p_1-ip_2)}{R+mc^2} \\ \dfrac{cp_3}{R+mc^2} \end{pmatrix}$$

$$\gamma_2 u_4{}^* = \sqrt{\frac{R+mc^2}{2R}} \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \dfrac{-c(p_x+ip_y)}{R+mc^2} \\ \dfrac{cp_z}{R+mc^2} \\ 0 \\ 1 \end{pmatrix} = \sqrt{\frac{R+mc^2}{2R}} \begin{pmatrix} -1 \\ 0 \\ \dfrac{cp_z}{R+mc^2} \\ \dfrac{-c(p_x+ip_y)}{R+mc^2} \end{pmatrix}$$

We note that u_1, u_2, u_3, and u_4 are obtained from the FW transformation

$$u_1 = \sqrt{\frac{R+mc^2}{2R}} \begin{pmatrix} 1 \\ 0 \\ \dfrac{cp_z}{R+mc^2} \\ \dfrac{c(p_x+ip_y)}{R+mc^2} \end{pmatrix}$$

$$u_2 = \sqrt{\frac{R+mc^2}{2R}} \begin{pmatrix} 0 \\ 1 \\ \dfrac{c(p_x-ip_y)}{R+mc^2} \\ -\dfrac{cp_z}{R+mc^2} \end{pmatrix}$$

$$u_3 = \sqrt{\frac{R+mc^2}{2R}} \begin{pmatrix} -\dfrac{cp_z}{R+mc^2} \\ \dfrac{c(p_x+ip_y)}{R+mc^2} \\ 1 \\ 0 \end{pmatrix}$$

$$u_4 = \sqrt{\frac{R+mc^2}{2R}} \begin{pmatrix} -\dfrac{c(p_x-ip_y)}{R+mc^2} \\ \dfrac{cp_z}{R+mc^2} \\ 0 \\ 1 \end{pmatrix}$$

When $p_1 = p_2 = p_3 = 0$

$$\gamma_2 u_1^* = -\begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}, \qquad \gamma_2 u_2^* = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} \qquad \gamma_2 u_3^* = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \qquad \gamma_2 u_4^* = -\begin{pmatrix} \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

((**Mathematica**))

```
Clear["Global`*"];
exp_* := exp /. {Complex[re_, im_] :> Complex[re, -im]};
σx = (0 1
      1 0); σy = (0 -ⅈ
                  ⅈ  0); σz = (1  0
                               0 -1);
I2 = IdentityMatrix[2];

αx = KroneckerProduct[σx, σx]; αy = KroneckerProduct[σx, σy];
αz = KroneckerProduct[σx, σz];
β = KroneckerProduct[σz, I2];

γ1 = -ⅈ β.αx // Simplify; γ2 = -ⅈ β.αy // Simplify;
 γ3 = -ⅈ β.αz // Simplify; γ4 = β;

Transpose[γ1] + γ1 // Simplify

{{0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}}

Transpose[γ2] - γ2 // Simplify

{{0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}}

Transpose[γ3] + γ3 // Simplify

{{0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}}

Transpose[γ4] - γ4 // Simplify

{{0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}}
```

Charge conjugate C

```
C1 = γ2.γ4 // Simplify
```

```
{{0, 0, 0, 1}, {0, 0, -1, 0}, {0, 1, 0, 0}, {-1, 0, 0, 0}}
```

```
C1 // MatrixForm
```

$$\begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}$$

```
γ1.C1 - C1.γ1 // Simplify
```

```
{{0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}}
```

```
γ2.C1 + C1.γ2 // Simplify
```

```
{{0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}}
```

```
γ3.C1 - C1.γ3 // Simplify
```

```
{{0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}}
```

```
γ4.C1 + C1.γ4 // Simplify
```

```
{{0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}}
```

```
Transpose[C1*] + C1
```

```
{{0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}}
```

```
Transpose[C1] + C1
```

```
{{0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}}
```

```
Inverse[C1] + C1
```

```
{{0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}}
```

23. Heisenberg's equation of motion (Heisenberg’s picture)

All operators are given by those in the Heisenberg picture. Here we omit the superscript (H).

$$\alpha_k{}^{(H)} = \alpha_k, \qquad \beta^{(H)} = \beta$$

$\alpha_k{}^{(H)}$ and $\beta^{(H)}$ must be regarded as dynamic variable.

The Hamiltonian

$$H = c\boldsymbol{\alpha}\cdot\boldsymbol{\pi} + eA_0 + \beta mc^2 = c\alpha_k\pi_k + eA_0 + \beta mc^2$$

with

$$\boldsymbol{\pi} = \boldsymbol{p} - \frac{e}{c}\boldsymbol{A}, \qquad A_\mu = (\boldsymbol{A}, iA_0)$$

$$\boldsymbol{B} = \nabla\times\boldsymbol{A}, \qquad E = -\frac{1}{c}\frac{\partial\boldsymbol{A}}{\partial t} - \nabla A_0$$

Heisenberg equation for the operator in the Heisenberg picture

$$\frac{d}{dt}O = \frac{i}{\hbar}[H,O] + \frac{\partial}{\partial t}O$$

(a)

$$\begin{aligned}
\frac{d}{dt}R_k &= \frac{i}{\hbar}[H,R_k] \\
&= \frac{i}{\hbar}c\alpha_j[\pi_j,R_k] + \frac{ie}{\hbar}[A_0,R_k] + \frac{i}{\hbar}[\beta mc^2,R_k] \\
&= \frac{i}{\hbar}c\alpha_j[p_j - \frac{e}{c}A_j,R_k] \\
&= \frac{i}{\hbar}c\alpha_j[p_{j\,j},R_k] \\
&= \frac{i}{\hbar}c\alpha_j\frac{\hbar}{i}\frac{\partial}{\partial R_j}R_k \\
&= c\alpha_j\delta_{j,k} \\
&= c\alpha_k
\end{aligned}$$

or

$$\frac{d}{dt}\boldsymbol{R} = c\boldsymbol{\alpha} = \boldsymbol{v}$$

(b)

$$\begin{aligned}
\frac{d}{dt}p_k &= \frac{i}{\hbar}[H, p_k] \\
&= \frac{i}{\hbar}c\alpha_j[\pi_j, p_k] + \frac{ie}{\hbar}[A_0, p_k] + \frac{i}{\hbar}[\beta mc^2, p_k] \\
&= \frac{i}{\hbar}c\alpha_j[p_j - \frac{e}{c}A_j, p_k] + \frac{ie}{\hbar}[A_0, p_k] \\
&= \frac{i}{\hbar}c\alpha_j \frac{e}{c}[p_k, A_j] - \frac{ie}{\hbar}[p_k, A_0] \\
&= \frac{i}{\hbar}c\alpha_j \frac{e}{c}\frac{\hbar}{i}\frac{\partial A_j}{\partial x_k} - \frac{ie}{\hbar}\frac{\hbar}{i}\frac{\partial A_0}{\partial x_k} \\
&= e\alpha_j \frac{\partial A_j}{\partial x_k} - \frac{ie}{\hbar}\frac{\partial A_0}{\partial x_k} \\
&= e\frac{\partial(\alpha_j A_j)}{\partial x_k} - e\frac{\partial A_0}{\partial x_k}
\end{aligned}$$

or

$$\frac{d}{dt}\boldsymbol{p} = e\nabla(\boldsymbol{\alpha}\cdot\boldsymbol{A}) - e\nabla A_0$$

(c)

$$\begin{aligned}
\frac{d}{dt}A_k &= \frac{i}{\hbar}[H, A_k] + \frac{\partial}{\partial t}A_k \\
&= \frac{i}{\hbar}c\alpha_j[\pi_j, A_k] + \frac{ie}{\hbar}[A_0, A_k] + \frac{i}{\hbar}[\beta mc^2, A_k] + \frac{\partial}{\partial t}A_k \\
&= \frac{i}{\hbar}c\alpha_j[p_j - \frac{e}{c}A_j, A_k] + \frac{ie}{\hbar}[A_0, A_k] + \frac{\partial}{\partial t}A_k \\
&= \frac{i}{\hbar}c\alpha_j[p_j, A_k] + \frac{\partial}{\partial t}A_k \\
&= \frac{i}{\hbar}c\alpha_j \frac{\hbar}{i}\frac{\partial A_k}{\partial x_j} + \frac{\partial}{\partial t}A_k \\
&= c\alpha_j \frac{\partial A_k}{\partial x_j} + \frac{\partial}{\partial t}A_k
\end{aligned}$$

or

$$\frac{d\boldsymbol{A}}{dt} = c(\boldsymbol{\alpha}\cdot\nabla)\boldsymbol{A} + \frac{\partial}{\partial t}\boldsymbol{A}.$$

(d)

$$\begin{aligned}
\frac{d\boldsymbol{\pi}}{dt} &= \frac{d}{dt}(\boldsymbol{p} - \frac{e}{c}\boldsymbol{A}) \\
&= e\nabla(\boldsymbol{\alpha}\cdot\boldsymbol{A}) - e\nabla A_0 - \frac{e}{c}[c(\boldsymbol{\alpha}\cdot\nabla)\boldsymbol{A} + \frac{\partial}{\partial t}\boldsymbol{A}] \\
&= e(-\frac{1}{c}\frac{\partial}{\partial t}\boldsymbol{A} - \nabla A_0) + e\boldsymbol{\alpha}\times(\nabla\times\boldsymbol{A}) \\
&= e(\boldsymbol{E} + \boldsymbol{\alpha}\times\boldsymbol{B}) \\
&= e(\boldsymbol{E} + \frac{\boldsymbol{v}}{c}\times\boldsymbol{B})
\end{aligned}$$

where

$$\nabla(\boldsymbol{\alpha}\cdot\boldsymbol{A}) - (\boldsymbol{\alpha}\cdot\nabla)\boldsymbol{A} = \boldsymbol{\alpha}\times(\nabla\times\boldsymbol{A})$$

(e)
We note that

$$\boldsymbol{\alpha}(H - eA_0) + (H - eA_0)\boldsymbol{\alpha} = 2c(\boldsymbol{p} - \frac{e}{c}\boldsymbol{A}) = 2c\boldsymbol{\pi}$$

Using this we obtain a quantum mechanical analogue of the Lorentz equation

$$\frac{d}{dt}\frac{1}{2}[\boldsymbol{v}(\frac{H - eA_0}{c^2}) + (\frac{H - eA_0}{c^2})\boldsymbol{v}] = \dot{\boldsymbol{\pi}} = e(\boldsymbol{E} + \boldsymbol{\alpha}\times\boldsymbol{B})$$

where

$$\frac{d\boldsymbol{R}}{dt} = c\boldsymbol{\alpha} = \boldsymbol{v},$$

$$\frac{d}{dt}\boldsymbol{\pi} = \frac{d}{dt}(\boldsymbol{p} - \frac{e}{c}\boldsymbol{A}) = e(\boldsymbol{E} + \boldsymbol{\alpha}\times\boldsymbol{B}).$$

If $H - eA_0 \approx \pm mc^2$, depending on whether the state is made of positive or negative energy solutions of the Dirac equation, we get the equation of motion under the Lorentz forc,

$$m\frac{d}{dt}\boldsymbol{v} = \pm e(\boldsymbol{E} + \frac{1}{c}\boldsymbol{v}\times\boldsymbol{B})$$

((**Note**))

$$\{\boldsymbol{\alpha}, H - eA_0\} = 2c(\boldsymbol{p} - \frac{e}{c}\boldsymbol{A})$$

or

$$\begin{aligned}\{\alpha_i, H - eA_0\} &= \{\alpha_i, c\alpha_j(p_j - \frac{e}{c}A_j) + \beta mc^2\} \\ &= c\{\alpha_i, \alpha_j\}(p_j - \frac{e}{c}A_j) \\ &= 2c\delta_{ij}(p_j - \frac{e}{c}A_j) \\ &= 2c(p_i - \frac{e}{c}A_i)\end{aligned}$$

where

$$\{\alpha_i, \beta\} = 0, \qquad \{\alpha_i, \alpha_j\} = 2\delta_{ij}.$$

(f)

$$\frac{d}{dt}(\boldsymbol{\Sigma} \cdot \boldsymbol{\pi}) = \frac{i}{\hbar}[H, \boldsymbol{\Sigma} \cdot \boldsymbol{\pi}] = e\boldsymbol{\Sigma} \cdot \boldsymbol{E}$$

where

$$H = c\boldsymbol{\alpha} \cdot \boldsymbol{\pi} + eA_0 + \beta mc^2 = c(-\gamma_5)\boldsymbol{\Sigma} \cdot \boldsymbol{\pi} + eA_0 + \beta mc^2$$

with

$$\alpha_k = i\gamma_4\gamma_k = -\gamma_5\Sigma_k, \quad \text{and} \quad [\gamma_5, \Sigma_k] = 0.$$

Then we get

$$\begin{aligned}
\frac{d}{dt}(\boldsymbol{\Sigma}\cdot\boldsymbol{\pi}) &= \frac{i}{\hbar}[H,\boldsymbol{\Sigma}\cdot\boldsymbol{\pi}] \\
&= \frac{i}{\hbar}[c(-\gamma_5)\boldsymbol{\Sigma}\cdot\boldsymbol{\pi} + eA_0 + \beta mc^2, \boldsymbol{\Sigma}\cdot\boldsymbol{\pi}] \\
&= \frac{ie}{\hbar}[A_0, \boldsymbol{\Sigma}\cdot\boldsymbol{\pi}] \\
&= -e\Sigma_k \frac{\partial A_0}{\partial x_k} \\
&= e\boldsymbol{\Sigma}\cdot\boldsymbol{E}
\end{aligned}$$

where

$$\begin{aligned}
[\beta, \boldsymbol{\Sigma}\cdot\boldsymbol{\pi}] &= [\beta, \Sigma_1\pi_1 + \Sigma_2\pi_2 + \Sigma_3\pi_3] \\
&= [\beta,\Sigma_1]\pi_1 + [\beta,\Sigma_2]\pi_2 + [\beta,\Sigma_3]\pi_3 \\
&= 0
\end{aligned}$$

$$\begin{aligned}
[\gamma_5\boldsymbol{\Sigma}\cdot\boldsymbol{\pi}, \boldsymbol{\Sigma}\cdot\boldsymbol{\pi}] &= \gamma_5(\boldsymbol{\Sigma}\cdot\boldsymbol{\pi})(\boldsymbol{\Sigma}\cdot\boldsymbol{\pi}) - (\boldsymbol{\Sigma}\cdot\boldsymbol{\pi})\gamma_5(\boldsymbol{\Sigma}\cdot\boldsymbol{\pi}) \\
&= 0
\end{aligned}$$

(g) Zitterbewegung ((Free particle))

$A_\mu = 0$.

$$\frac{d\boldsymbol{p}}{dt} = 0 \qquad\qquad \boldsymbol{p} = \text{constant}$$

The Hamiltonian of free particle is given by

$$H = c\boldsymbol{\alpha}\cdot\boldsymbol{p} + \beta mc^2$$

Heisenberg's equation for the operator $\boldsymbol{\alpha}$,

$$\begin{aligned}\frac{d\boldsymbol{\alpha}}{dt} &= \frac{1}{c}\frac{d\boldsymbol{v}}{dt} \\ &= \frac{i}{\hbar}[H,\boldsymbol{\alpha}] \\ &= \frac{i}{\hbar}(H\boldsymbol{\alpha} - \boldsymbol{\alpha}H) \\ &= -\frac{i}{\hbar}(H\boldsymbol{\alpha} + \boldsymbol{\alpha}H - 2H\boldsymbol{\alpha}) \\ &= -\frac{2i}{\hbar}(c\boldsymbol{p} - H\boldsymbol{\alpha})\end{aligned}$$

where

$$H\boldsymbol{\alpha} + \boldsymbol{\alpha}H = 2c\boldsymbol{p}$$

((Note))

$$\{H,\alpha_k\} = cp_i\{\alpha_i,\alpha_k\} + mc^2\{\beta,\alpha_i\} = 2cp_i$$

Since H = const., this equation has a simple solution:

$$\frac{d\boldsymbol{\alpha}}{dt} = \frac{2i}{\hbar}H(\boldsymbol{\alpha} - H^{-1}c\boldsymbol{p})$$

or

$$\boldsymbol{\alpha} = \frac{\boldsymbol{v}(t)}{c} = H^{-1}c\boldsymbol{p} + \exp(\frac{2i}{\hbar}Ht)[\boldsymbol{\alpha}(0) - H^{-1}c\boldsymbol{p}]$$

or

$$\boldsymbol{v}(t) = H^{-1}c^2\boldsymbol{p} + ce^{2iHt/\hbar}[\boldsymbol{\alpha}(0) - H^{-1}c\boldsymbol{p}]$$

This equation can be integrated:

$$\boldsymbol{r}(t) = \boldsymbol{r}(0) + H^{-1}c^2\boldsymbol{p}t + \frac{\hbar c}{2iH}(e^{2iHt/\hbar} - 1)[\boldsymbol{\alpha}(0) - H^{-1}c\boldsymbol{p}]$$

The first two terms on the right-hand side describe simply the uniform motion of a free particle. The last term is a feature of relativistic quantum mechanics and connotes a high-frequency vibration (Zitterbewegung) of the particle with frequency $mc^2/\hbar$ and amplitude $\hbar/(mc)$, the Compton wavelength of the particle.

(h) Free particles (continued)

For a free particle Hamiltonian,

$$\{\beta, H\} = \{\beta, c\boldsymbol{\alpha}\cdot\boldsymbol{p} + \beta mc^2\} = 2mc^2\beta^2 + cp_k\{\beta, \alpha_k\} = 2mc^2$$

and

$$\begin{aligned}\{\gamma_5, H\} &= \{\gamma_5, c\boldsymbol{\alpha}\cdot\boldsymbol{p} + \beta mc^2\} \\ &= cp_k\{\gamma_5, \alpha_k\} + mc^2\{\gamma_5, \beta\} \\ &= -cp_k\{\gamma_5, \gamma_5\Sigma_k\} \\ &= -2cp_k\Sigma_k\end{aligned}$$

Hence, in a state of energy E, the operator β has the expectation value

$$<\beta> = \frac{mc^2}{E} = +\sqrt{1-\left(\frac{cp}{E}\right)^2}$$

Similarly,

$$<\gamma_5> = -\frac{cp}{E} <\boldsymbol{\Sigma}\cdot\hat{\boldsymbol{p}}>$$

where $\hat{\boldsymbol{p}}$ is the unit vector of $\boldsymbol{p}$. The operator γ_5 is called the chirality.

(i) Lorentz force

$A_0 = 0$, $\boldsymbol{A} \neq 0$ (vector potential)

The Hamiltonian H is given by

$$H = c\boldsymbol{\alpha}\cdot(\boldsymbol{p} - \frac{e}{c}\boldsymbol{A}) + \beta mc^2 .$$

$$\frac{d}{dt}\boldsymbol{\Sigma} = \frac{i}{\hbar}[H, \boldsymbol{\Sigma}]$$

$$\alpha_k = -\Sigma_k\gamma_5 = -\gamma_5\Sigma_k , \qquad [\beta, \Sigma_k] = 0$$

$$\Sigma_k = -i\gamma_i\gamma_j \qquad (i, j, k\text{: cyclic})$$

$$[\gamma_5, \Sigma_k] = 0\,, \quad , \qquad [\gamma_5, \alpha_k] = 0\,, \quad [\beta, \gamma_5] = 0$$

$$[\Sigma_i, \Sigma_j] = 2i\Sigma_k\,, \qquad \Sigma_i\Sigma_j = -\Sigma_j\Sigma_i = i\Sigma_k \quad (i, j, \text{ and } k\text{; cyclic})$$

$$[\gamma_5\Sigma_k, \Sigma_j] = \gamma_5\Sigma_k\Sigma_j - \Sigma_j\gamma_5\Sigma_k = \gamma_5[\Sigma_k, \Sigma_j]\,.$$

Using the Mathematica, we get

$$\begin{aligned}
[H, \Sigma_1] &= [c\alpha_k(p_k - \frac{e}{c}A_k) + \beta mc^2, \Sigma_1] \\
&= [-c\gamma_5\Sigma_k(p_k - \frac{e}{c}A_k), \Sigma_i] \\
&= 2ic[\alpha_2(p_3 - \frac{e}{c}A_3) - \alpha_3(p_2 - \frac{e}{c}A_2)] \\
&= 2ic[\boldsymbol{\alpha} \times (\boldsymbol{p} - \frac{e}{c}\boldsymbol{A})]_1
\end{aligned}$$

or

$$[H, \boldsymbol{\Sigma}] = 2ic[\boldsymbol{\alpha} \times (\boldsymbol{p} - \frac{e}{c}\boldsymbol{A})]$$

leading to the Heisenberg's equation,

$$\frac{d\boldsymbol{\Sigma}}{dt} = \frac{i}{\hbar}[H, \boldsymbol{\Sigma}] = -\frac{2c}{\hbar}[\boldsymbol{\alpha} \times (\boldsymbol{p} - \frac{e}{c}\boldsymbol{A})]$$

So we have

$$\begin{aligned}
H\frac{d\boldsymbol{\Sigma}}{dt} + \frac{d\boldsymbol{\Sigma}}{dt}H &= -\frac{2c^2}{\hbar}[\boldsymbol{\alpha} \cdot (\boldsymbol{p} - \frac{e}{c}\boldsymbol{A})][\boldsymbol{\alpha} \times (\boldsymbol{p} - \frac{e}{c}\boldsymbol{A})] \\
&\quad + \boldsymbol{\alpha} \times (\boldsymbol{p} - \frac{e}{c}\boldsymbol{A})][\boldsymbol{\alpha} \cdot (\boldsymbol{p} - \frac{e}{c}\boldsymbol{A})] \\
&= 2ec\boldsymbol{\Sigma} \times \boldsymbol{B}
\end{aligned}$$

In the relativistic approximation, $H \approx mc^2$. Then we have

$$\frac{d\boldsymbol{\Sigma}}{dt} = \frac{2ec}{2mc^2}\boldsymbol{\Sigma}\times\boldsymbol{B} = \frac{e}{mc}\boldsymbol{\Sigma}\times\boldsymbol{B}$$

Since

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

$$\frac{d\boldsymbol{\sigma}}{dt} = \frac{e}{mc}\boldsymbol{\sigma}\times\boldsymbol{B}$$

For the one electron spin operator

$$\boldsymbol{S} = \frac{\hbar}{2}\boldsymbol{\sigma}$$

$$\frac{d\boldsymbol{S}}{dt} = \frac{e}{mc}\boldsymbol{S}\times\boldsymbol{B} = \boldsymbol{\mu}\times\boldsymbol{B}$$

or

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

24. Central force problem: hydrogen atom

The Hamiltonian is given by

$$H = c\boldsymbol{\alpha}\cdot\boldsymbol{p} + \beta mc^2 + eA_0$$

where

$$A_\mu = (\boldsymbol{A}, iA_0)$$

with

$$\boldsymbol{A} = 0 \qquad eA_0 = V(r) \qquad \text{(spherical symmetry)}$$

(a) The commutation relation between J_3 and H

$$[H, J_3] = 0$$

((**Proof**))

$$
\begin{aligned}
[H - eA_0, L_3] &= [c\boldsymbol{\alpha}\cdot\boldsymbol{p} + \beta mc^2, L_3] \\
&= c[p_k, L_3]\alpha_k + mc^2[\beta, L_3] \\
&= c[p_k, x_1 p_2 - x_2 p_1]\alpha_k \\
&= c[p_1, x_1 p_2 - x_2 p_1]\alpha_1 + c[p_2, x_1 p_2 - x_2 p_1]\alpha_2 \\
&= \frac{\hbar}{i} cp_2\alpha_1 - \frac{\hbar}{i} cp_1\alpha_2 \\
&= \frac{\hbar}{i} c(p_2\alpha_1 - p_1\alpha_2) \\
&= \frac{c\hbar}{i}(\boldsymbol{\alpha}\times\boldsymbol{p})_3
\end{aligned}
$$

or

$$
[H, L_3] = -ic\hbar(\boldsymbol{\alpha}\times\boldsymbol{p})_3 + [eA_0, L_3] = -ic\hbar(\boldsymbol{\alpha}\times\boldsymbol{p})_3
$$

since

$$
\begin{aligned}
[eA_0, L_3] &= [eA_0, xp_y - yp_x] \\
&= -x[p_y, eA_0] + y[p_x, eA_0] \\
&= -x\frac{\hbar}{i}\frac{\partial}{\partial y} eA_0 + y\frac{\hbar}{i}\frac{\partial}{\partial x} eA_0 \\
&= 0
\end{aligned}
$$

where

$$
A_0 = A_0(r), \qquad r = \sqrt{x^2 + y^2 + z^2}
$$

$$
x\frac{\partial}{\partial y}A_0 - y\frac{\partial}{\partial x}A_0 = (x\frac{\partial r}{\partial y} - y\frac{\partial r}{\partial x})\frac{\partial A_0}{\partial r} = (\frac{xy}{r} - \frac{xy}{r})\frac{\partial A_0}{\partial r} = 0
$$

Similarly

$$
\begin{aligned}
[H - eA_0, \Sigma_3] &= [c\alpha_k p_k + \beta mc^2, \Sigma_3] \\
&= [c\alpha_k p_k, \Sigma_3] + [\beta mc^2, \Sigma_3] \\
&= -cp_k \gamma_5 [\Sigma_k, \Sigma_3] \\
&= -cp_1 \gamma_5 [\Sigma_1, \Sigma_3] - cp_2 \gamma_5 [\Sigma_2, \Sigma_3] \\
&= 2icp_1 \gamma_5 \Sigma_2 - 2icp_2 \gamma_5 \Sigma_1 \\
&= 2ic(\alpha_1 p_2 - \alpha_2 p_1) \\
&= 2ic(\boldsymbol{\alpha} \times \boldsymbol{p})_3
\end{aligned}
$$

or

$$
\begin{aligned}
[H, \Sigma_3] &= 2ic(\boldsymbol{\alpha} \times \boldsymbol{p})_3 + [eA_0, \Sigma_3] \\
&= 2ic(\boldsymbol{\alpha} \times \boldsymbol{p})_3
\end{aligned}
$$

or

$$
[H, \frac{\hbar}{2}\Sigma_3] = i c\hbar (\boldsymbol{\alpha} \times \boldsymbol{p})_3
$$

where

$$
\alpha_k = -\gamma_5 \Sigma_k, \quad [\gamma_5, \Sigma_k] = 0, \quad [\beta, \Sigma_k] = 0, \quad \{\gamma_5, \beta\} = 0
$$

$$
[\alpha_k, \Sigma_1] = [-\gamma_5 \Sigma_k, \Sigma_1] = -\gamma_5 [\Sigma_k, \Sigma_1]
$$

$$
[\Sigma_i, \Sigma_j] = 2i\Sigma_k \qquad (i, j, k; \text{ cyclic})
$$

Thus we have

$$
[H, J_3] = [H, L_3 + \frac{\hbar}{2}\Sigma_3] = -ic\hbar(\boldsymbol{\alpha} \times \boldsymbol{p})_3 + ic\hbar(\boldsymbol{\alpha} \times \boldsymbol{p})_3 = 0
$$

Similarly, we have

$$
[H, J_1] = 0, \quad [H, J_2] = 0.
$$

or

$[H, \boldsymbol{J}] = 0$.

(b) Definition of the operator K and the commutation relation $[K,H]=0$

First we show that

$$[H,\beta\boldsymbol{\Sigma}\cdot\boldsymbol{J}]=\frac{\hbar}{2}[H,\beta]$$

where

$$[H,\boldsymbol{J}]=0 \qquad \text{and} \qquad [\beta,\boldsymbol{\Sigma}]=0$$

((**Proof**))

$$\begin{aligned}[H,\beta\boldsymbol{\Sigma}\cdot\boldsymbol{J}]&=H\beta(\boldsymbol{\Sigma}\cdot\boldsymbol{J})-\beta(\boldsymbol{\Sigma}\cdot\boldsymbol{J})H\\&=[H,\beta](\boldsymbol{\Sigma}\cdot\boldsymbol{J})+\beta[H,\boldsymbol{\Sigma}]\cdot\boldsymbol{J}\\&=-2c\beta(\boldsymbol{\alpha}\cdot\boldsymbol{p})(\boldsymbol{\Sigma}\cdot\boldsymbol{J})+2ic\beta(\boldsymbol{\alpha}\times\boldsymbol{p})\cdot\boldsymbol{J}\end{aligned}$$

Here we note that

$$[H,\beta]=[c\boldsymbol{\alpha}\cdot\boldsymbol{p},\beta]=c\boldsymbol{\alpha}\cdot\boldsymbol{p}\beta-\beta c\boldsymbol{\alpha}\cdot\boldsymbol{p}=-2\beta c\boldsymbol{\alpha}\cdot\boldsymbol{p}$$

$$[H,\boldsymbol{\Sigma}]=2ic(\boldsymbol{\alpha}\times\boldsymbol{p})$$

$$\begin{aligned}(\boldsymbol{\alpha}\cdot\boldsymbol{p})(\boldsymbol{\Sigma}\cdot\boldsymbol{J})&=-\gamma_5(\boldsymbol{\Sigma}\cdot\boldsymbol{p})(\boldsymbol{\Sigma}\cdot\boldsymbol{J})\\&=-\gamma_5[\boldsymbol{p}\cdot\boldsymbol{J}+i\boldsymbol{\Sigma}\cdot(\boldsymbol{p}\times\boldsymbol{J})]\\&=-\gamma_5\boldsymbol{p}\cdot\boldsymbol{J}+i\boldsymbol{\alpha}\cdot(\boldsymbol{p}\times\boldsymbol{J})\end{aligned}$$

Then we have

$$\begin{aligned}[H,\beta\boldsymbol{\Sigma}\cdot\boldsymbol{J}]&=-2c\beta[-\gamma_5\boldsymbol{p}\cdot\boldsymbol{J}+i\boldsymbol{\alpha}\cdot(\boldsymbol{p}\times\boldsymbol{J})]+2ic\beta(\boldsymbol{\alpha}\times\boldsymbol{p})\cdot\boldsymbol{J}\\&=2c\beta\gamma_5\boldsymbol{p}\cdot\boldsymbol{J}\\&=2c\beta\gamma_5\boldsymbol{p}\cdot(\boldsymbol{L}+\frac{\hbar}{2}\boldsymbol{\Sigma})\\&=c\hbar\beta\gamma_5\boldsymbol{p}\cdot\boldsymbol{\Sigma}\\&=-c\hbar\beta\boldsymbol{\alpha}\cdot\boldsymbol{p}\\&=\frac{\hbar}{2}[H,\beta]\end{aligned}$$

where

$$(\boldsymbol{\alpha}\times\boldsymbol{p})\cdot\boldsymbol{J}=\boldsymbol{\alpha}\cdot(\boldsymbol{p}\times\boldsymbol{J})$$

Then we define the operator K as

$$\begin{aligned}K &= \beta\boldsymbol{\Sigma}\cdot\boldsymbol{J} - \frac{\hbar}{2}\beta \\ &= \beta(\boldsymbol{\Sigma}\cdot\boldsymbol{J} - \frac{\hbar}{2}) \\ &= \beta(\boldsymbol{\Sigma}\cdot\boldsymbol{L} + \frac{\hbar}{2}\boldsymbol{\Sigma}^2 - \frac{\hbar}{2}) \\ &= \beta(\boldsymbol{\Sigma}\cdot\boldsymbol{L} + \hbar)\end{aligned}$$

where

$$\boldsymbol{J} = \boldsymbol{L} + \frac{\hbar}{2}\boldsymbol{\Sigma}$$

Then K commutes with H,

$$[K, H] = 0.$$

This also implies that

$$[K^2, H] = 0.$$

25. Commutation relations (continued)

(i) $[\beta, \boldsymbol{J}] = 0$

$$[\beta, J_1] = [\beta, L_1 + \frac{\hbar}{2}\Sigma_1] = \frac{\hbar}{2}[\beta, \Sigma_1] = 0$$

(ii) $[\beta\boldsymbol{\Sigma}\cdot\boldsymbol{J}, \boldsymbol{J}] = 0$

$$
\begin{aligned}
[\beta\boldsymbol{\Sigma}\cdot\boldsymbol{L},J_1] &= [\beta\sum_1 L_1+\beta\sum_2 L_2+\beta\sum_3 L_3, L_1+\frac{\hbar}{2}\Sigma_1] \\
&= [\beta\sum_1 L_1+\beta\sum_2 L_2+\beta\sum_3 L_3, L_1]+[\beta\sum_1 L_1+\beta\sum_2 L_2+\beta\sum_3 L_3,\frac{\hbar}{2}\Sigma_1] \\
&= -\beta\sum_2[L_1,L_2]+\beta\sum_3[L_3,L_1]+\frac{\hbar}{2}[\beta\sum_2 L_2,\Sigma_1]+\frac{\hbar}{2}[\beta\sum_3 L_3,\Sigma_1] \\
&= -i\hbar\beta\sum_2 L_3+i\hbar\beta\sum_3 L_2-\frac{\hbar}{2}L_2\beta[\sum_1,\Sigma_2]+\frac{\hbar}{2}L_3\beta[\sum_3,\Sigma_1] \\
&= -i\hbar\beta\sum_2, L_3+i\hbar\beta\sum_3 L_2-i\hbar L_2\beta\sum_3+i\hbar L_3\beta\Sigma_2 \\
&= 0
\end{aligned}
$$

since

$$[\beta,\sum_k]=0$$

(iii) $[\beta\boldsymbol{\Sigma}\cdot\boldsymbol{J},\boldsymbol{J}]=0$

$$
\begin{aligned}
[\beta\boldsymbol{\Sigma}\cdot\boldsymbol{J},J_1] &= [\beta\boldsymbol{\Sigma}\cdot(\boldsymbol{L}+\frac{\hbar}{2}\Sigma),J_1] \\
&= [\beta\boldsymbol{\Sigma}\cdot\boldsymbol{L},J_1]+\frac{\hbar}{2}[\beta\sum^2,J_1] \\
&= \frac{\hbar}{2}[3\beta,J_1] \\
&= 0
\end{aligned}
$$

or

$$[\beta\boldsymbol{\Sigma}\cdot\boldsymbol{J},\boldsymbol{J}]=0$$

which leads to

$$[K,\boldsymbol{J}]=[\beta(\boldsymbol{\Sigma}\cdot\boldsymbol{L}+\hbar),\boldsymbol{J}]=0$$

26. K^2 and J^2

$$
\begin{aligned}
K^2 &= \beta(\boldsymbol{\Sigma}\cdot\boldsymbol{L}+\hbar)\beta(\boldsymbol{\Sigma}\cdot\boldsymbol{L}+\hbar) \\
&= (\boldsymbol{\Sigma}\cdot\boldsymbol{L})(\boldsymbol{\Sigma}\cdot\boldsymbol{L})+2\hbar\boldsymbol{\Sigma}\cdot\boldsymbol{L}+\hbar^2 \\
&= \boldsymbol{L}^2+i\sum\cdot(\boldsymbol{L}\times\boldsymbol{L})+2\hbar\boldsymbol{\Sigma}\cdot\boldsymbol{L}+\hbar^2 \\
&= \boldsymbol{L}^2+\hbar\boldsymbol{\Sigma}\cdot\boldsymbol{L}+\hbar^2
\end{aligned}
$$

since

$$[\beta, \Sigma_k] = 0 .$$

We note that

$$\begin{aligned}
\boldsymbol{J}^2 &= (\boldsymbol{L} + \frac{\hbar}{2}\boldsymbol{\Sigma}) \cdot (\boldsymbol{L} + \frac{\hbar}{2}\boldsymbol{\Sigma}) \\
&= \boldsymbol{L}^2 + \frac{\hbar}{4}\boldsymbol{\Sigma}^2 + \hbar\boldsymbol{\Sigma} \cdot \boldsymbol{L} \\
&= \boldsymbol{L}^2 + \frac{3\hbar^2}{4} + \hbar\boldsymbol{\Sigma} \cdot \boldsymbol{L}
\end{aligned}$$

Thus we obtain

$$K^2 = J^2 + \frac{\hbar^2}{4}$$

Since $[K^2, H] = 0$, we also have the commutation relation

$$[\boldsymbol{J}^2, H] = 0$$

27. Simultaneous eigenket

For an electron in a central potential, we can conduct a simultaneous eigenfunction of H, *K*, $\boldsymbol{J}^2$, and J_3,

$$H\psi = E\psi , \qquad K\psi = -\kappa\hbar\psi ,$$

$$\boldsymbol{J}^2\psi = \hbar^2 j(j+1)\psi , \qquad J_3\psi = j_3\hbar\psi$$

$$P\psi = \pm\psi$$

since

$$[H, K] = 0 , \quad [H, J_3] = 0 , \quad [H, J^2] = 0 , \quad [P, H] = 0$$

We also note that

$$K^2 = \boldsymbol{J}^2 + \frac{\hbar^2}{4}$$

This implies that

$$K^2\psi = \hbar^2\kappa^2\psi = [\hbar^2 j(j+1) + \frac{\hbar^2}{4}]\psi = \hbar^2(j+\frac{1}{2})^2\psi$$

or

$$\kappa^2\psi = [j(j+1) + \frac{1}{4}]\psi =^2 (j+\frac{1}{2})^2\psi$$

So we must have

$$\kappa = \pm(j+\frac{1}{2}),$$

Note that j is a half-integer and κ is an integer ($\kappa = \pm1, \pm2, \ldots$). So κ has integer eigenvalues not zero.

28. Operator *K*

We now consider the matrix of *K*.

$$\begin{aligned} K &= \beta(\boldsymbol{\Sigma}\cdot\boldsymbol{L}+\hbar) \\ &= \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} \boldsymbol{\sigma}\cdot\boldsymbol{L}+\hbar & 0 \\ 0 & \boldsymbol{\sigma}\cdot\boldsymbol{L}+\hbar \end{pmatrix} \\ &= \begin{pmatrix} \boldsymbol{\sigma}\cdot\boldsymbol{L}+\hbar & 0 \\ 0 & -(\boldsymbol{\sigma}\cdot\boldsymbol{L}+\hbar) \end{pmatrix} \end{aligned}$$

The wave function ψ is a simultaneous function of K, $\boldsymbol{J}^2$, and J_3,

$$\psi = \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix}$$

Then we have

$$K\psi = -\hbar\kappa\psi$$

or

$$\begin{pmatrix} \boldsymbol{\sigma}\cdot\boldsymbol{L}+\hbar & 0 \\ 0 & -(\boldsymbol{\sigma}\cdot\boldsymbol{L}+\hbar) \end{pmatrix}\begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix} = -\hbar\kappa\begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix}$$

or

$$(\boldsymbol{\sigma}\cdot\boldsymbol{L}+\hbar)\psi_A = -\hbar\kappa\psi_A, \qquad (\boldsymbol{\sigma}\cdot\boldsymbol{L}+\hbar)\psi_B = \hbar\kappa\psi_B$$

or

$$(\boldsymbol{\sigma}\cdot\boldsymbol{L})\psi_A = -\hbar(\kappa+1)\psi_A, \qquad (\boldsymbol{\sigma}\cdot\boldsymbol{L})\psi_B = \hbar(\kappa-1)\psi_B$$

29. Operators $\boldsymbol{J}^2$

$$\boldsymbol{J}^2\psi = \hbar^2 j(j+1)\psi$$

$$\boldsymbol{J} = \boldsymbol{L}+\frac{\hbar}{2}\boldsymbol{\Sigma} = \begin{pmatrix} \boldsymbol{L}+\frac{\hbar}{2}\boldsymbol{\sigma} & 0 \\ 0 & \boldsymbol{L}+\frac{\hbar}{2}\boldsymbol{\sigma} \end{pmatrix}$$

$$\begin{aligned}\boldsymbol{J}^2 &= \begin{pmatrix} \boldsymbol{L}+\frac{\hbar}{2}\boldsymbol{\sigma} & 0 \\ 0 & \boldsymbol{L}+\frac{\hbar}{2}\boldsymbol{\sigma} \end{pmatrix}\begin{pmatrix} \boldsymbol{L}+\frac{\hbar}{2}\boldsymbol{\sigma} & 0 \\ 0 & \boldsymbol{L}+\frac{\hbar}{2}\boldsymbol{\sigma} \end{pmatrix} \\ &= \begin{pmatrix} \left(\boldsymbol{L}+\frac{\hbar}{2}\boldsymbol{\sigma}\right)^2 & 0 \\ 0 & \left(\boldsymbol{L}+\frac{\hbar}{2}\boldsymbol{\sigma}\right)^2 \end{pmatrix}\end{aligned}$$

Then we get

$$\boldsymbol{J}^2\psi_{A,B} = \hbar^2 j(j+1)\psi_{A,B}$$

or

$$\left(\boldsymbol{L}+\frac{\hbar}{2}\boldsymbol{\sigma}\right)^2\psi_A = \hbar^2 j(j+1)\psi_A, \qquad \left(\boldsymbol{L}+\frac{\hbar}{2}\boldsymbol{\sigma}\right)^2\psi_B = \hbar^2 j(j+1)\psi_B$$

30. Operator J_z

$$J_3\psi = (L_3+\frac{\hbar}{2}\Sigma_3)\psi = \begin{pmatrix} L_3+\frac{\hbar}{2}\sigma_3 & 0 \\ 0 & L_3+\frac{\hbar}{2}\sigma_3 \end{pmatrix}\begin{pmatrix}\psi_A \\ \psi_B\end{pmatrix} = j_3\hbar\begin{pmatrix}\psi_A \\ \psi_B\end{pmatrix}$$

or

$$(L_3 + \frac{\hbar}{2}\sigma_3)\psi_A = j_3\hbar\psi_A, \qquad (L_3 + \frac{\hbar}{2}\sigma_3)\psi_B = j_3\hbar\psi_A$$

31 The operator $\boldsymbol{L}^2$

Since $[H, \boldsymbol{L}^2] \neq 0$, ψ is not the eigenfunction.

$$\boldsymbol{L}^2 = \boldsymbol{J}^2 - \hbar\boldsymbol{\Sigma}\cdot\boldsymbol{L} - \frac{3\hbar^2}{4}$$

we have

$$\boldsymbol{L}^2\psi = \begin{pmatrix} \boldsymbol{J}^2 - \hbar\boldsymbol{\sigma}\cdot\boldsymbol{L} - \frac{3\hbar^2}{4} & 0 \\ 0 & \boldsymbol{J}^2 - \hbar\boldsymbol{\sigma}\cdot\boldsymbol{L} - \frac{3\hbar^2}{4} \end{pmatrix}\begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix}$$

Then we get

$$\begin{aligned}(\boldsymbol{J}^2 - \hbar\boldsymbol{\sigma}\cdot\boldsymbol{L} - \frac{3\hbar^2}{4})\psi_A &= [\boldsymbol{J}^2 - \hbar(\boldsymbol{\sigma}\cdot\boldsymbol{L} + \hbar) + \frac{\hbar^2}{4})\psi_A \\ &= [\hbar^2 j(j+1) + \hbar^2\kappa + \frac{\hbar^2}{4}]\psi_A \\ &= \hbar^2 l_A(l_A+1)\psi_A\end{aligned}$$

where

$$j(j+1) + \kappa + \frac{1}{4} = l_A(l_A+1)$$

Similarly,

$$\begin{aligned}(\boldsymbol{J}^2 - \hbar\boldsymbol{\sigma}\cdot\boldsymbol{L} - \frac{3\hbar^2}{4})\psi_B &= [\boldsymbol{J}^2 - \hbar(\boldsymbol{\sigma}\cdot\boldsymbol{L} + \hbar) + \frac{\hbar^2}{4}]\psi_B \\ &= [\hbar^2 j(j+1) - \hbar^2\kappa + \frac{\hbar^2}{4}]\psi_B \\ &= \hbar^2 l_B(l_B+1)\psi_B\end{aligned}$$

with

$$j(j+1)-\kappa+\frac{1}{4}=l_B(l_B+1)$$

Thus ψ_A and ψ_B are separately the eigenfunctions of $\boldsymbol{L}^2$. These eigenvalues are denoted by $l_A(l_A+1)\hbar^2$ and $\hbar^2 l_B(l_B+1)$, respectively.

Using these two equations, we can determine l_A and l_B for the given eigenvalue κ.

((**Nonrelativistic case**))

$n = 1$; $l = 0$

$D_0 \times D_{1/2} = D_{1/2}$ $\quad$ (j = 1/2)

$n = 2$; $l = 0, 1$

$D_0 \times D_{1/2} = D_{1/2}$ $\quad$ (j = 1/2)
$D_1 \times D_{1/2} = D_{3/2} + D_{1/2}$ $\quad$ (j = 3/2, 1/2)

$n = 3$; $l = 0, 1, 2$

$D_0 \times D_{1/2} = D_{1/2}$ $\quad$ (j = 1/2)
$D_1 \times D_{1/2} = D_{3/2} + D_{1/2}$ $\quad$ (j = 3/2, 1/2)
$D_2 \times D_{1/2} = D_{5/2} + D_{3/2}$ $\quad$ (j = 5/2, 3/2)

(a) For j = 1/2,

$$\kappa=\pm(j+\frac{1}{2})=\pm 1.$$

(i) $\kappa=1$, l_A = 1, and l_B = 0.
(ii) $\kappa=-1$, l_A = 0 and l_B = 1.

(b) For a half integer j,

$$\kappa=\pm(j+\frac{1}{2}).$$

(i) $\kappa=j+\frac{1}{2}$, $\quad l_A=j+\frac{1}{2}$, $\quad l_B=j-\frac{1}{2}$

(ii) $\kappa = -(j+\frac{1}{2})$,` $l_A = j - \frac{1}{2}$, $l_B = j + \frac{1}{2}$

32. Normalized spin angular function

Spin orbit coupling

$$D_l \times D_{1/2} = D_{l+1/2} + D_{l-1/2}$$

For $j = l + 1/2$,

$$y_l^{j=l+1/2, j_3} = \sqrt{\frac{l + j_3 + 1/2}{2l+1}} Y_l^{j_3-1/2} \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \sqrt{\frac{l - j_3 + 1/2}{2l+1}} Y_l^{j_3+1/2} \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$= \frac{1}{\sqrt{2l+1}} \begin{pmatrix} \sqrt{l + j_3 + \frac{1}{2}} Y_l^{j_3-1/2} \\ \sqrt{l - j_3 + \frac{1}{2}} Y_l^{j_3+1/2} \end{pmatrix}$$

For $j = l - 1/2$,

$$y_l^{j=l-1/2, j_3} = -\sqrt{\frac{l - j_3 + 1/2}{2l+1}} Y_l^{j_3-1/2} \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$+ \sqrt{\frac{l + j_3 + 1/2}{2l+1}} Y_l^{j_3+1/2} \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$= \frac{1}{\sqrt{2l+1}} \begin{pmatrix} -\sqrt{l - j_3 + \frac{1}{2}} Y_l^{j_3-1/2} \\ \sqrt{l + j_3 + \frac{1}{2}} Y_l^{j_3+1/2} \end{pmatrix}$$

33. Radial wave functions

(a) For $\kappa = j + \frac{1}{2}$, $l_A = j + \frac{1}{2}$, $l_B = j - \frac{1}{2}$

$$\psi = \begin{pmatrix} g(r) y_{l_A = j+\frac{1}{2}}^{j, j_3} \\ i f(r) y_{l_B = j-\frac{1}{2}}^{j, j_3} \end{pmatrix}$$

(b) For $\kappa = -(j+\frac{1}{2})$, $l_A = j - \frac{1}{2}$, $l_B = j + \frac{1}{2}$

$$\psi = \begin{pmatrix} f(r) y_{l_A = j-\frac{1}{2}}^{j,j_3} \\ i g(r) y_{l_B = j+\frac{1}{2}}^{j,j_3} \end{pmatrix}$$

The parity of $y_{l_A = j-\frac{1}{2}}^{j,j_3}$ is given by $(-1)^{l_A}$, while the parity of $y_{l_B = j+\frac{1}{2}}^{j,j_3}$ is given by $(-1)^{l_B}$. Theses parities are different, since $l_B - l_A = \pm 1$. The radial functions *f* and *g* depend on *κ*. The factor *i* multiplying *f* and *g* is inserted to make *f* and *g* real for bound-state.

((**Note**))

$$\psi_A(-\boldsymbol{r},t) = (-1)^{l_A}\psi_A(\boldsymbol{r},t) = \pm\psi_A(\boldsymbol{r},t)$$

$$\psi_B(-\boldsymbol{r},t) = (-1)^{l_B}\psi_B(\boldsymbol{r},t) = \mp\psi_B(\boldsymbol{r},t)$$

Thus we have

$$(-1)^{l_A} = (-1)^{l_B+1}$$

Thus we get the relation

$$l_A - l_B = \pm 1.$$

Table-1

κ	l_A	l_B
$\kappa = -(j+\frac{1}{2})$	$l_A = j - \frac{1}{2}$	$l_B = j + \frac{1}{2}$
$\kappa = (j+\frac{1}{2})$	$l_A = j + \frac{1}{2}$	$l_B = j - \frac{1}{2}$

Table-2

$j = \frac{1}{2}$

$\kappa = 1$,	$l_A = 1$,	$l_B = 0$
$\kappa = -1$,	$l_A = 0$,	$l_B = 1$

$j = \frac{3}{2}$

$\kappa = 2$, $l_A = 2$, $l_B = 1$

$\kappa = -2$, $l_A = 1$, $l_B = 2$

$j = \frac{5}{2}$

$\kappa = 3$, $l_A = 3$, $l_B = 2$

$\kappa = -3$, $l_A = 2$, $l_B = 3$

34. Expression of the two-component wave function

For a fixed κ [= j+1/2, or -(j+1/2)] we assume that the wave function is given by

$$\psi = \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix} = \begin{pmatrix} f(r) y_{l_A}^{j,j_3} \\ ig(r) y_{l_B}^{j,j_3} \end{pmatrix}$$

This function satisfies the Dirac equation given by

$$c(\boldsymbol{\sigma} \cdot \boldsymbol{p})\psi_B = (E - V(r) - mc^2)\psi_A,$$

$$c(\boldsymbol{\sigma} \cdot \boldsymbol{p})\psi_A = (E - V(r) - mc^2)\psi_B$$

We note that

$$\begin{aligned} \boldsymbol{\sigma} \cdot \boldsymbol{p} &= \frac{1}{r^2}(\boldsymbol{\sigma} \cdot \boldsymbol{r})(\boldsymbol{\sigma} \cdot \boldsymbol{r})(\boldsymbol{\sigma} \cdot \boldsymbol{p}) \\ &= \frac{1}{r^2}(\boldsymbol{\sigma} \cdot \boldsymbol{r})[\boldsymbol{r} \cdot \boldsymbol{p} + \boldsymbol{\sigma} \cdot (\boldsymbol{r} \times \boldsymbol{p})] \\ &= \frac{1}{r^2}(\boldsymbol{\sigma} \cdot \boldsymbol{r})(\boldsymbol{r} \cdot \boldsymbol{p} + i\boldsymbol{\sigma} \cdot \boldsymbol{L}) \\ &= \frac{1}{r^2}(\boldsymbol{\sigma} \cdot \boldsymbol{r})(-i\hbar r\frac{\partial}{\partial r} + i\boldsymbol{\sigma} \cdot \boldsymbol{L}) \end{aligned}$$

where

$$(\boldsymbol{\sigma} \cdot \boldsymbol{r})(\boldsymbol{\sigma} \cdot \boldsymbol{r}) = r^2 + i\boldsymbol{\sigma} \cdot (\boldsymbol{r} \times \boldsymbol{r}) = r^2$$

$$\boldsymbol{r} \cdot \boldsymbol{p} = \frac{\hbar}{i} r \frac{\partial}{\partial r}$$

$$\boldsymbol{p} = \frac{\hbar}{i}\nabla = \frac{\hbar}{i}(\boldsymbol{e}_r \frac{\partial}{\partial r} + \boldsymbol{e}_\theta \frac{1}{r}\frac{\partial}{\partial \theta} + \boldsymbol{e}_\phi \frac{1}{r\sin\theta}\frac{\partial}{\partial \phi})$$

For two arbitrary vectors $\boldsymbol{A}$ and $\boldsymbol{B}$,

$$(\boldsymbol{\sigma}\cdot\boldsymbol{A})(\boldsymbol{\sigma}\cdot\boldsymbol{B}) = (\boldsymbol{A}\cdot\boldsymbol{B})\hat{1} + i\boldsymbol{\sigma}\cdot(\boldsymbol{A}\times\boldsymbol{B})$$

Then we get

$$\begin{aligned}
(\boldsymbol{\sigma}\cdot\boldsymbol{p})\psi_B &= i(\boldsymbol{\sigma}\cdot\boldsymbol{p}) f(r) y_{l_B}^{j,j_3} \\
&= \frac{i}{r^2}(\boldsymbol{\sigma}\cdot\boldsymbol{r})(-i\hbar r\frac{\partial}{\partial r} + i\boldsymbol{\sigma}\cdot\boldsymbol{L}) f(r) y_{l_B}^{j,j_3} \\
&= (\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}})[-\hbar\frac{df}{dr} - \frac{(1-\kappa)\hbar}{r} f] y_{l_B}^{j,j_3} \\
&= -\hbar\frac{df}{dr} y_{l_A}^{j,j_3} - \frac{(1-\kappa)\hbar}{r} f y_{l_A}^{j,j_3}
\end{aligned}$$

where

$$(\boldsymbol{\sigma}\cdot\boldsymbol{L})\psi_B = \hbar(\kappa-1)\psi_B, \qquad (\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}}) y_{l_B}^{j,j_3} = y_{l_A}^{j,j_3}.$$

Similarly, we get

$$\begin{aligned}
(\boldsymbol{\sigma}\cdot\boldsymbol{p})\psi_A &= (\boldsymbol{\sigma}\cdot\boldsymbol{p}) g y_{l_A}^{j,j_3} \\
&= \frac{1}{r^2}(\boldsymbol{\sigma}\cdot\boldsymbol{r})(-i\hbar r\frac{\partial}{\partial r} + i\boldsymbol{\sigma}\cdot\boldsymbol{L}) g y_{l_A}^{j,j_3} \\
&= \frac{\hbar}{r^2}(\boldsymbol{\sigma}\cdot\boldsymbol{r})[-ir\frac{dg}{dr} - i(\kappa+1)g] y_{l_A}^{j,j_3} \\
&= -[i\hbar\frac{dg}{dr} + i(\kappa+1)\hbar g] y_{l_B}^{j,j_3} \\
&= i\hbar\frac{dg}{dr} y_{l_B}^{j,j_3} + i\frac{(\kappa+1)\hbar}{r} g y_{l_B}^{j,j_3}
\end{aligned}$$

where

$$(\boldsymbol{\sigma}\cdot\boldsymbol{L})\psi_A = -\hbar(\kappa+1)\psi_A, \qquad (\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}}) y_{l_A}^{j,j_3} = -y_{l_B}^{j,j_3}$$

35. The operator $(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}})$

(a) $\{P, \boldsymbol{\Sigma}\cdot\hat{\boldsymbol{r}}\} = 0$

with $\quad P = \beta\pi$

((**Proof**))

$$\begin{aligned}\{P, \boldsymbol{\Sigma}\cdot\hat{\boldsymbol{r}}\} &= \{\beta\pi, \boldsymbol{\Sigma}\cdot\hat{\boldsymbol{r}}\} \\ &= \beta\pi\boldsymbol{\Sigma}\cdot\hat{\boldsymbol{r}} + \boldsymbol{\Sigma}\cdot\hat{\boldsymbol{r}}\beta\pi \\ &= \beta\boldsymbol{\Sigma}\cdot\pi\hat{\boldsymbol{r}} + \boldsymbol{\Sigma}\cdot\beta\hat{\boldsymbol{r}}\pi \\ &= \beta\boldsymbol{\Sigma}\cdot\pi\hat{\boldsymbol{r}} - \boldsymbol{\Sigma}\cdot\beta\pi\hat{\boldsymbol{r}} \\ &= [\beta, \boldsymbol{\Sigma}]\cdot\pi\hat{\boldsymbol{r}} \\ &= 0\end{aligned}$$

or

$$\begin{pmatrix} \pi(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}}) + (\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}})\pi & 0 \\ 0 & -\pi(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}}) - \pi(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}}) \end{pmatrix} = 0$$

or

$$\pi(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}}) + (\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}})\pi = 0$$

where, $P = \beta\pi$ and $\pi\hat{\boldsymbol{r}} + \hat{\boldsymbol{r}}\pi = 0$. Thus we have

$\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}}$ is odd under the parity.

(b) $\quad (\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}})^2 = 1$

((**Proof**))

$$(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}})(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}}) = \hat{\boldsymbol{r}}\cdot\hat{\boldsymbol{r}} + i\boldsymbol{\sigma}\cdot(\hat{\boldsymbol{r}}\times\hat{\boldsymbol{r}}) = 1$$

(c) $\quad [J_3, \boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}}] = 0$

((**Proof**))

$$J_3 = L_3 + S_3 = L_3 + \frac{\hbar}{2}\sigma_3$$

$$L_3 = \frac{\hbar}{i}\frac{\partial}{\partial\phi}$$

$$\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}} = \sigma_1\sin\theta\cos\phi + \sigma_2\sin\theta\sin\phi + \sigma_3\cos\theta$$

Then we can evaluate the commutation relation

$$[J_3, \boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}}] = [L_3, \boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}}] + \frac{\hbar}{2}[\sigma_3, \boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}}]$$

$$\begin{aligned}
[L_3, \boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}}]\psi &= L_3[(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}})\psi] - (\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}})L_3\psi \\
&= \frac{\hbar}{i}\frac{\partial}{\partial\phi}[(\sigma_1\sin\theta\cos\phi + \sigma_2\sin\theta\sin\phi + \sigma_3\cos\theta)\psi \\
&\quad -(\sigma_1\sin\theta\cos\phi + \sigma_2\sin\theta\sin\phi + \sigma_3\cos\theta)L_3\psi \\
&= \frac{\hbar}{i}\psi\frac{\partial}{\partial\phi}(\sigma_1\sin\theta\cos\phi + \sigma_2\sin\theta\sin\phi + \sigma_3\cos\theta) \\
&\quad +(\sigma_1\sin\theta\cos\phi + \sigma_2\sin\theta\sin\phi + \sigma_3\cos\theta)L_3\psi \\
&\quad -(\sigma_1\sin\theta\cos\phi + \sigma_2\sin\theta\sin\phi + \sigma_3\cos\theta)L_3\psi \\
&= -i\hbar\psi(-\sigma_1\sin\theta\sin\phi + \sigma_2\sin\theta\cos\phi)
\end{aligned}$$

or

$$[L_3, \boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}}] = i\hbar\sigma_1\sin\theta\sin\phi - i\hbar\sigma_2\sin\theta\cos\phi$$

We also have

$$\begin{aligned}
[\frac{\hbar}{2}\sigma_3, \boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}}] &= \frac{\hbar}{2}[\sigma_3, \sigma_1\sin\theta\cos\phi + \sigma_2\sin\theta\sin\phi + \sigma_3\cos\theta] \\
&= \frac{\hbar}{2}[\sigma_3, \sigma_1]\sin\theta\cos\phi - \frac{\hbar}{2}[\sigma_2, \sigma_3]\sin\theta\sin\phi \\
&= i\hbar\sigma_2\sin\theta\cos\phi - i\hbar\sigma_1\sin\theta\sin\phi
\end{aligned}$$

Thus we have

$$[J_3, \boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}}] = 0$$

36. Evaluation of $(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}})y_{l_A}^{j,j_3}$ and $(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}})y_{l_B}^{j,j_3}$

(a)

$$[J_3, \boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}}]y_{l_A}^{j,j_3} = 0$$

or

$$[J_3(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}})y_{l_A}^{j,j_3} = (\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}})J_3 y_{l_A}^{j,j_3} = j_3(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}})y_{l_A}^{j,j_3}$$

which means that $(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}})y_{l_A}^{j,j_3}$ is the eigenfunction of J_3 with the eigenvalue j_3.

(b)

$$\pi(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}})y_{l_A}^{j,j_3}=-(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}})\pi y_{l_A}^{j,j_3}=(-1)^{l_A+1}(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}})y_{l_A}^{j,j_3}$$

$$\pi(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}})y_{l_B}^{j,j_3}=-(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}})\pi y_{l_B}^{j,j_3}=(-1)^{l_B+1}(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}})y_{l_B}^{j,j_3}$$

leading to the relation

$$(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}})y_{l_A}^{j,j_3}=cy_{l_B}^{j,j_3}, \qquad (\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}})y_{l_B}^{j,j_3}=cy_{l_A}^{j,j_3}$$

where c is constants. We note that

$$(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}})^2y_{l_A}^{j,j_3}=c(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}})y_{l_B}^{j,j_3}=c^2y_{l_A}^{j,j_3}=y_{l_A}^{j,j_3}$$

since

$$(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}})^2=1$$

Then we get $c=\pm 1$. Here we choose c = -1.

$$(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}})y_{l_A}^{j,j_3}=-y_{l_B}^{j,j_3}, \qquad (\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}})y_{l_B}^{j,j_3}=-y_{l_A}^{j,j_3}$$

((**Note**)) In the non-relativistic quantum mechanics, it is well known that

$$\hat{\pi}|l,m\rangle=(-1)^l|l,m\rangle$$

37. Radial wave function in hydrogen atom

Now we solve the Dirac equation as

$$c(\boldsymbol{\sigma}\cdot\boldsymbol{p})\psi_B=(E-V(r)-mc^2)\psi_A,$$

or

$$c(\boldsymbol{\sigma}\cdot\boldsymbol{p})\psi_B=-c\hbar\frac{df}{dr}y_{l_A}^{j,j_3}-\frac{(1-\kappa)c\hbar}{r}fy_{l_A}^{j,j_3}=(E-V(r)-mc^2)gy_{l_A}^{j,j_3}$$

or

$$-\hbar c\frac{df}{dr}-\frac{(1-\kappa)\hbar c}{r}f=(E-V(r)-mc^2)g$$

Similarly,

$$c(\boldsymbol{\sigma}\cdot\boldsymbol{p})\psi_A = (E - V(r) + mc^2)\psi_B$$

or

$$\hbar c\frac{dg}{dr} + \frac{(1+\kappa)\hbar c}{r}g = (E - V(r) + mc^2)f$$

Introducing

$$F(r) = rf(r), \qquad G(r) = rg(r)$$

then we have a radial equations,

$$\hbar c(\frac{dF}{dr} - \frac{\kappa}{r}F) = -(E - V(r) - mc^2)G$$

$$\hbar c(\frac{dG}{dr} + \frac{\kappa}{r}G) = (E - V(r) + mc^2)F$$

We assume that $V(r)$ is given by a Coulomb potential

$$V(r) = -\frac{Ze^2}{r}$$

We put

$$\alpha_1 = \frac{mc^2 + E}{\hbar c}, \qquad \alpha_2 = \frac{mc^2 - E}{\hbar c}$$

$$\gamma = \frac{Ze^2}{\hbar c} = Z\alpha, \qquad \rho = \sqrt{\alpha_1\alpha_2}\,r, \qquad \mu = \sqrt{\frac{\alpha_2}{\alpha_1}}$$

where α is the fine structure constant,

$$\alpha = \frac{e^2}{\hbar c} = 7.29735257 \text{ x } 10^{-3}, \qquad \frac{1}{\alpha} = 137.035999074(44).$$

Then we get the coupled equations we need to solve,

$$(\frac{d}{d\rho}-\frac{\kappa}{\rho})F-(\mu-\frac{\gamma}{\rho})G=0$$

$$(\frac{d}{d\rho}+\frac{\kappa}{\rho})G-(\frac{1}{\mu}+\frac{\gamma}{\rho})F=0$$

The analysis of the radial equation proceeds as usual.

$\rho\to\infty$,

$$\frac{dF}{d\rho}=\mu G\,, \qquad \frac{dG}{d\rho}=\sqrt{\frac{\alpha_1}{\alpha_2}}F$$

$$\frac{d^2F}{d\rho^2}=\sqrt{\frac{\alpha_2}{\alpha_1}}\frac{dG}{d\rho}=\sqrt{\frac{\alpha_2}{\alpha_1}}\sqrt{\frac{\alpha_1}{\alpha_2}}F=F$$

Similarly,

$$\frac{d^2G}{d\rho^2}=G$$

$$F=e^{-\rho}\,, \qquad G=e^{-\rho}$$

We assume that

$$F=e^{-\rho}\rho^s\sum_{m=0}a_m\rho^m$$

$$G=e^{-\rho}\rho^s\sum_{m=0}b_m\rho^m$$

We solve the problem using a series expension method. These series forms are substituted into the coupled differential equation. We use the Mathematica to determine the value of *s* and the recursion relation. The results are as follows.

38 Indicial equation to determine the value of s

$$(s-\kappa)a_0+\gamma b_0=0$$
$$-\gamma a_0+(s+\kappa)b_0=0$$

or

$$\begin{pmatrix} s-\kappa & \gamma \\ -\gamma & s+\kappa \end{pmatrix}\begin{pmatrix} a_0 \\ b_0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

Since a_0 and b_0 are not zero (non-trivial solution), the determinant of the matrix should be equal to zero.

$$s = \pm\sqrt{\kappa^2 - \gamma^2}$$

Note that

$$s^2 = \kappa^2 - \gamma^2 > \min(\kappa^2) - \gamma^2 = 1 - (Z\alpha)^2$$

So we get approximately $s > 1$, or s<-1. However, we must require that

$$\int |\psi(r)|^2 r^2 dr < \infty$$

The requirement amounts to

$$\int |f(r)|^2 r^2 dr = \int \frac{|F(r)|^2}{r^2} r^2 dr = \int |F(r)|^2 dr \approx \int |F(\rho)|^2 d\rho < \infty$$

$$\int |g(r)|^2 r^2 dr = \int \frac{|G(r)|^2}{r^2} r^2 dr = \int |G(r)|^2 dr \approx \int |G(\rho)|^2 d\rho < \infty$$

Around the origin,

$$F \approx \rho^s, \qquad G \approx \rho^s$$

Then we have

$$\int |F(\rho)|^2 d\rho \approx \int \rho^{2s} d\rho = \frac{\rho^{2s+1}}{2s+1}$$

$$\int |G(\rho)|^2 d\rho \approx \int \rho^{2s} d\rho = \frac{\rho^{2s+1}}{2s+1}$$

So in order to get the finite value of the probability near the origin, it is required that

$$s > -\frac{1}{2}$$

So we need to take

$$s = \sqrt{\kappa^2 - \gamma^2} = \sqrt{(j+\frac{1}{2})^2 - Z^2\alpha^2}$$

39. Mathematica (series expansion method)

```
Clear["Global`*"];

eq1 = D[F[ρ], ρ] - κ/ρ F[ρ] - (μ - γ/ρ) G[ρ]; eq2 = D[G[ρ], ρ] + κ/ρ G[ρ] - (1/μ + γ/ρ) F[ρ];

rule1 = {F → (Exp[-#] #^s (Sum[A[k] #^k, {k, 0, 10}]) &)}; rule2 = {G → (Exp[-#] #^s (Sum[B[k] #^k, {k, 0, 10}]) &)};

eq11 = eq1 /. rule1 /. rule2 // Expand; eq21 = eq2 /. rule1 /. rule2 // Expand;
eq12 = eq11 Exp[ρ] ρ^(1-s) // Simplify; eq22 = eq21 Exp[ρ] ρ^(1-s) // Simplify;
```

Determinastin of s

```
list1 = Table[{n, Coefficient[eq12, ρ, n]}, {n, 0, 2}] // Simplify; list1 // TableForm
```

0	$s A[0] - \kappa A[0] + \gamma B[0]$
1	$-A[0] + (1 + s - \kappa) A[1] - \mu B[0] + \gamma B[1]$
2	$-A[1] + (2 + s - \kappa) A[2] - \mu B[1] + \gamma B[2]$

```
list2 = Table[{n, Coefficient[eq22, ρ, n]}, {n, 0, 2}] // Simplify; list2 // TableForm
```

0	$-\gamma A[0] + (s + \kappa) B[0]$
1	$-\frac{A[0]}{\mu} - \gamma A[1] - B[0] + B[1] + s B[1] + \kappa B[1]$
2	$\frac{-A[1] + \mu (-\gamma A[2] - B[1] + (2 + s + \kappa) B[2])}{\mu}$

Determination of recursion formula

```
rule3 = {F → (Exp[-#] #^s (Sum[A[n] #^n, {n, q-3, q+3}]) &)}; rule4 = {G → (Exp[-#] #^s (Sum[B[n] #^n, {n, q-3, q+3}]) &)};

eq13 = eq1 /. rule3 /. rule4 // Expand; eq23 = eq2 /. rule3 /. rule4 // Expand;
eq14 = eq13 Exp[ρ] ρ^(4-q-s) // Simplify; eq24 = eq23 Exp[ρ] ρ^(4-q-s) // Simplify;

list3 = Table[{n, Coefficient[eq14, ρ, n]}, {n, 2, 4}] // Simplify; list3 // TableForm

2    -A[-2 + q] + (-1 + q + s - κ) A[-1 + q] - μ B[-2 + q] + γ B[-1 + q]
3    -A[-1 + q] + (q + s - κ) A[q] - μ B[-1 + q] + γ B[q]
4    -A[q] + (1 + q + s - κ) A[1 + q] - μ B[q] + γ B[1 + q]

list4 = Table[{n, Coefficient[ eq24, ρ, n]}, {n, 2, 4}] // Expand; list4 // TableForm

2    -A[-2+q]/μ - γ A[-1 + q] - B[-2 + q] - B[-1 + q] + q B[-1 + q]
     + s B[-1 + q] + κ B[-1 + q]
3    -A[-1+q]/μ - γ A[q] - B[-1 + q] + q B[q]
     + s B[q] + κ B[q]
4    -A[q]/μ - γ A[1 + q] - B[q] + B[1 + q] + q B[1 + q] + s B[1 + q] + κ B[1 + q]

sq1 = Coefficient[eq12, ρ, 0]; sq2 = Coefficient[eq22, ρ, 0];

M1 = ( D[sq1, A[0]]  D[sq1, B[0]]
       D[sq2, A[0]]  D[sq2, B[0]] ); Det[M1]
s^2 + γ^2 - κ^2
```

40. Recirsion relation

(i) The second recursion relations

$$(s+1-\kappa)a_1 - a_0 + \gamma b_1 - \mu b_0 = 0$$

$$(s+1+\kappa)b_1 - b_0 - \gamma a_1 - \frac{1}{\mu}a_0 = 0$$

(ii) The recursion relations (the general case)

$$(s+q-\kappa)a_q - a_{q-1} + \gamma b_q - \mu b_{q-1} = 0$$

$$(s+q+\kappa)b_q - b_{q-1} - \gamma a_q - \frac{1}{\mu}a_{q-1} = 0$$

The functions F and G would increase exponentially as $\rho \to \infty$ if the power series do not terminate. Assuming that the two series terminates with the same power, there must be exist n_r with the property. For $q = n_r$, we assume that

$$a_{n_r+1} = b_{n_r+1} = 0, \qquad a_{n_r} \neq 0, \qquad b_{n_r} \neq 0$$

Then we get

$$a_{n_r} = -\mu b_{n_r} \qquad (1)$$

From the recursion relation (in general)

$$(s+q-\kappa)a_q + \gamma b_q = a_{q-1} + \mu b_{q-1}$$

$$\mu[(s+q+\kappa)b_q - \gamma a_q] = a_{q-1} + \mu b_{q-1}$$

we get the relation

$$\mu[(s+q+\kappa)b_q - \gamma a_q] = (s+q-\kappa)a_q + \gamma b_q$$

or

$$[\mu(s+q+\kappa)-\gamma]b_q = (s+q-\kappa+\mu\gamma)a_q. \qquad (2)$$

or

$$C_q = \frac{a_q}{s+q+\kappa-\dfrac{\gamma}{\mu}} = \frac{b_q}{\dfrac{1}{\mu}(s+q-\kappa)+\gamma}$$

for $q = n_r, n_{r-1}, ..., 0$.

41. Derivation of the energy eigenvalue

From Eqs.(1) and (2) with $q = n_r$, we have

$$[\mu(s+n_r+\kappa)-\gamma]b_{n_r} = (s+n_r-\kappa+\mu\gamma)a_{n_r} = -\mu(s+n_r-\kappa+\mu\gamma)b_{n_r}$$

or

$$[\mu(s+n_r+\kappa)-\gamma] = -\mu(s+n_r-\kappa+\mu\gamma)$$

or

$$s+n_r = \gamma\frac{1-\mu^2}{2\mu} = \gamma\frac{(\alpha_1-\alpha_2)}{2\sqrt{\alpha_1\alpha_2}}$$

or

$$2\sqrt{\alpha_1\alpha_2}(s+n_r)=\gamma(\alpha_1-\alpha_2)$$

Noting that

$$\alpha_1-\alpha_2=\frac{2E}{\hbar c}, \qquad \sqrt{\alpha_1\alpha_2}=\frac{\sqrt{m^2c^4-E^2}}{\hbar c}$$

we have the energy eigenvalue as

$$\sqrt{m^2c^4-E^2}(s+n_r)=\gamma E$$

or

$$E=\frac{mc^2}{\sqrt{1+\frac{\gamma^2}{(n_r+s)^2}}}=\frac{mc^2}{\sqrt{1+\frac{Z^2\alpha^2}{(n-j-\frac{1}{2}+\sqrt{(j+\frac{1}{2})^2-Z^2\alpha^2})^2}}}$$

This is famous fine structure formula for the hydrogen atom. The quantum numbers j and nr assume the values

$$j=\frac{1}{2},\frac{3}{2},\frac{5}{2},\dots . \qquad n_r = 0,\ 1,\ 2,\ 3,\dots$$

The principal quantum number n of the nonrelativistic theory of the hydrogen atom is related to nr and j by

$$n=j+\frac{1}{2}+n_r$$

$n = 1$

$n_r = 0,\ j=\frac{1}{2}$

($l = 0$, $s = 1/2$) $j = 1/2$ $1\ {}^2S_{1/2}$ $\kappa=-1$

$n = 2$

$n_r = 0,\ j=\frac{3}{2}$

($l = 1$, $s = 1/2$) $j = 3/2$ $2\ {}^2P_{3/2}$ $\kappa=-2$

$n_r = 1, \;\; j = \dfrac{1}{2}$

($l = 0$, $s = 1/2$)	$j = 1/2$	$2\,^2S_{1/2}$	$\kappa = -1$
($l = 1$, $s = 1/2$)	$j = 1/2$	$2\,^2P_{1/2}$	$\kappa = 1$

$n = 3$

$n_r = 0, \;\; j = \dfrac{5}{2}$

($l = 2$, $s = 1/2$	$j = 5/2$	$3\,^2D_{5/2}$)	$\kappa = -3$

$n_r = 1, \;\; j = \dfrac{3}{2}$

($l = 1$, $s = 1/2$	$j = 3/2$	$3\,^2P_{3/2}$)	$\kappa = -2$
($l = 2$, $s = 1/2$	$j = 3/2$	$3\,^2D_{3/2}$)	$\kappa = 2$

$n_r = 2, \;\; j = \dfrac{1}{2}$

($l = 0$, $s = 1/2$	$j = 1/2$	$3\,^2S_{1/2}$)	$\kappa = -1$
($l = 1$, $s = 1/2$	$j = 1/2$	$3\,^2P_{1/2}$)	$\kappa = 1$

Table-2

$j = \dfrac{1}{2}$

$\kappa = 1$,	$l = 1$
$\kappa = -1$,	$l = 0$

$j = \dfrac{3}{2}$

$\kappa = 2$,	$l = 2$
$\kappa = -2$,	$l = 1$

$j = \dfrac{5}{2}$

$\kappa = 3$,	$l = 3$
$\kappa = -3$,	$l = 2$

Table 3 Notation in the nonrelativistic case

$n = 1$

$l = 0$,	$s = 1/2$	$j = 1/2$	$1\,^2S_{1/2}$

$n = 2$

$l = 0$,	$s = 1/2$	$j = 1/2$	$2\ ^2S_{1/2}$
$l = 1$,	$s = 1/2$	$j = 3/2$	$2\ ^2P_{3/2}$
$l = 1$,	$s = 1/2$	$j = 1/2$	$2\ ^2P_{1/2}$

$n = 3$

$l = 0$,	$s = 1/2$	$j = 1/2$	$3\ ^2S_{1/2}$
$l = 1$,	$s = 1/2$	$j = 3/2$	$3\ ^2P_{3/2}$
$l = 1$,	$s = 1/2$	$j = 1/2$	$3\ ^2P_{1/2}$
$l = 2$,	$s = 1/2$	$j = 5/2$	$3\ ^2D_{5/2}$
$l = 2$,	$s = 1/2$	$j = 3/2$	$3\ ^2D_{3/2}$

42. Energy levels

The energy ΔE

$$\Delta E = \frac{mc^2}{\sqrt{1 + \frac{Z^2\alpha^2}{(n - j - \frac{1}{2} + \sqrt{(j + \frac{1}{2})^2 - Z^2\alpha^2})^2}}} - mc^2$$

can be expanded by using a Taylor expansion in a power of $Z^2\alpha^2$.

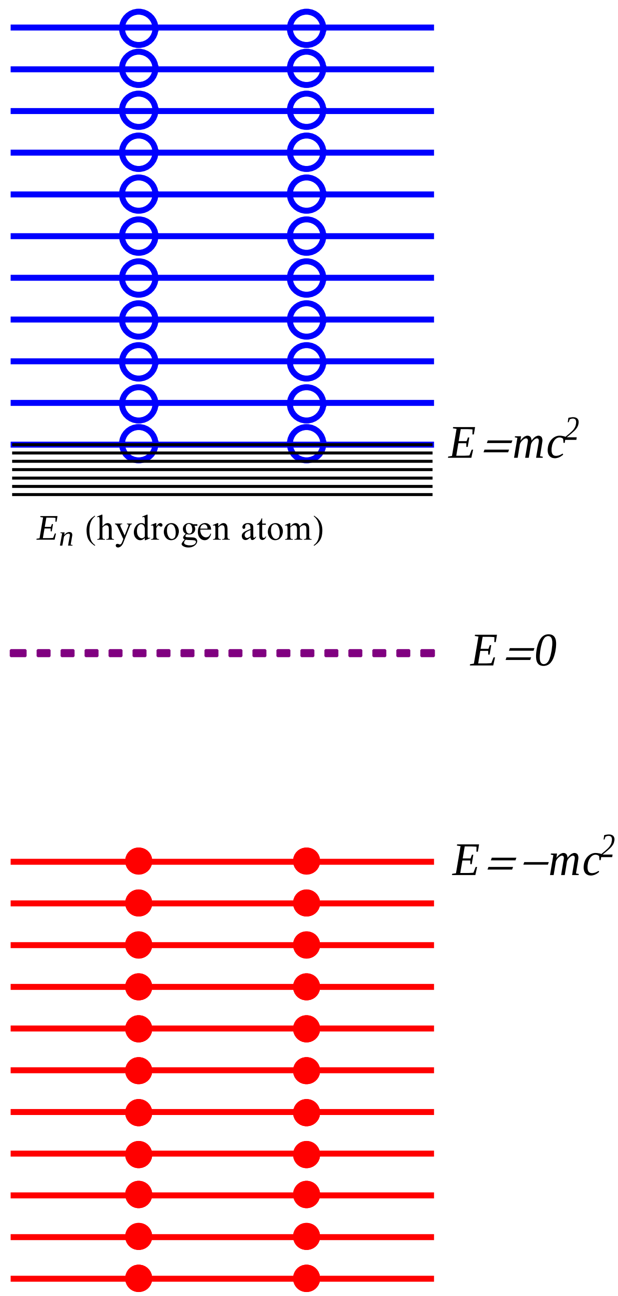


Fig. The energy levels of electron in the hydrogen atom (in the relativistic quantum mechanics)

Using the Mathematica, we have

$$
\begin{aligned}
\Delta E &= E - mc^2 \\
&= -\frac{mc^2}{2n^2}(Z\alpha)^2 + \frac{mc^2(6j+3-8n)}{8(1+2j)n^4}(Z\alpha)^4 + ... \\
&= -\frac{mc^2}{2n^2}(Z\alpha)^2 - \frac{mc^2}{2n^3}(Z\alpha)^4\left(\frac{1}{j+\frac{1}{2}} - \frac{3}{4n}\right) + ...
\end{aligned}
$$

The first tem is the non-relativistic limit

$$
-\frac{mc^2}{2n^2}(Z\alpha)^2 = -\frac{13.6057Z^2}{n^2}\ [\text{eV}]
$$

The second term is the relativistic correction to ΔE.

The principal quantum number n are n = 1, 2, 3, 4, … and $j+1/2 \le n$. There is the degeneracy between 2 $^2S_{1/2}$ ans 2 $^2P_{1/2}$.states (similarly 3 $^2S_{1/2}$ ans 3 $^2P_{1/2}$, 3 $^2P_{3/2}$ ans 3 $^2D_{3/2}$) persists in the eaxct solution to the Dirac equation. This degeneracy is lifted by the Lamb shift due to the coupling of electron to the zero-point fluctuation of the radiation field.

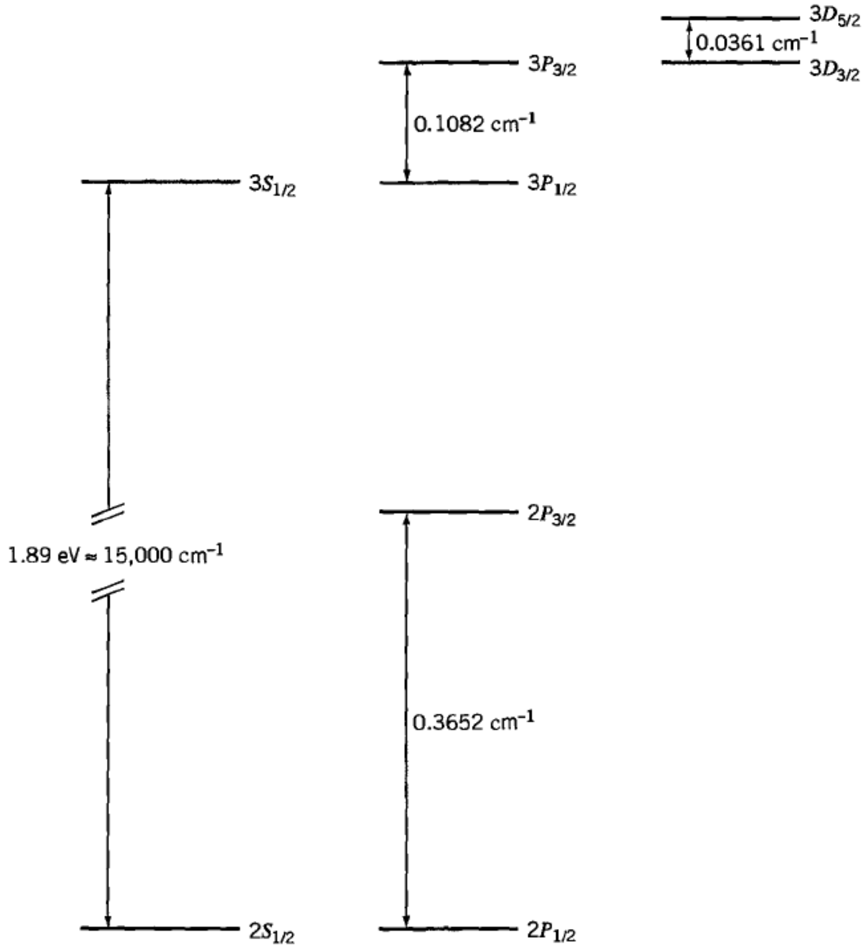


Fig. Detail of an energy-level diagram for the hydrogen atom. The manifolds of the n = 2 and n = 3 levels are shown, based on the Dirac theory, without radiative corrections (Lamb shifts) or hyperfine splittings. The energy differences are given in the units of cm^{-1}. 1eV = 8065.56 cm^{-1}. ((**Merzbacher, Quantum Mechanics**)

((**Mathematica**))
The energy is in the units of cm^{-1}; $E(erg)/(2\pi\hbar c)$.
1 eV = 8065.56 cm^{-1}

```
Clear["Global`*"];
rule1 = {c → 2.99792 × 10^10, ℏ → 1.054571628 10^-27,
   me → 9.10938215 10^-28, eV → 1.602176487 × 10^-12,
   α → 7.2973525376 × 10^-3, Z → 1};
```

$$E0 = \frac{me\,c^2}{\sqrt{1 + \frac{Z^2\,\alpha^2}{\left(n1 - j1 - \frac{1}{2} + \sqrt{\left(j1 + \frac{1}{2}\right)^2 - Z^2\,\alpha^2}\right)^2}}} - me\,c^2;$$

$$\frac{1\,eV}{2\,\pi\,\hbar\,c} \;//.\; rule1$$

8065.56

```
Series[E0, {α, 0, 4}] //
 FullSimplify[#, {j1 > 0, n1 > 0}] &
```

$$-\frac{\left(c^2\,me\,Z^2\right)\,\alpha^2}{2\,n1^2} + \frac{c^2\,me\,(3 + 6\,j1 - 8\,n1)\,Z^4\,\alpha^4}{8\,(1 + 2\,j1)\,n1^4} + O[\alpha]^5$$

```
E1[n_, j_] := E0 / (2 π ℏ c) /. {n1 → n, j1 → j} //. rule1

E1[3, 5 / 2] - E1[3, 3 / 2]
```

0.0360719

```
E1[3, 3 / 2] - E1[3, 1 / 2]
```

0.108219

```
E1[2, 3 / 2] - E1[2, 1 / 2]
```

0.365241

```
E1[3, 1 / 2] - E1[2, 1
   / 2]
```

15 241.6

43. Wave function for the ground state

Suppose that $n_r = 0$. Then we have

$$a_1 = b_1 = 0\,, \qquad a_0 \neq 0\,, \qquad\qquad b_0 \neq 0$$

From the recursion relation,

$$-a_0 - \mu b_0 = 0$$

or

$$a_0 = -\mu b_0 \tag{1}$$

From the indicial equation

$$-\gamma a_0 + (s + \kappa) b_0 = 0 \tag{2}$$

Using these two equations, we have

$$\frac{a_0}{b_0} = \frac{s + \kappa}{\gamma} = -\mu < 0$$

where

$$s = \sqrt{\kappa^2 - \gamma^2} < |\kappa|$$

Then we have

$$s + \kappa < 0 \qquad \text{and} \qquad 0 < s < |\kappa|$$

or

$$\kappa < -s < 0$$

The absence of the $\kappa > 0$ state for $n_r = 0$ corresponds to the familiar rule in relativistic quantum mechanics.

<u>Ground state:</u>

$$n = j + \frac{1}{2} + n_r$$

with $n = 1$. $n_r = 0$, $j = 1/2$.

$$E = \frac{mc^2}{\sqrt{1+\frac{Z^2\alpha^2}{1-Z^2\alpha^2}}} = \frac{mc^2}{\sqrt{\frac{1}{1-Z^2\alpha^2}}} = mc^2\sqrt{1-Z^2\alpha^2} \qquad \text{(ground state energy)}$$

$$\frac{a_0}{b_0} = -\mu = -\sqrt{\frac{mc^2+E}{mc^2-E}} = -\frac{1+\sqrt{1-Z^2\alpha^2}}{Z\alpha} \approx -\frac{2}{Z\alpha}$$

$$\rho = \frac{\sqrt{\alpha_1\alpha_2}\,r}{\hbar c} = \frac{mc}{\hbar}(Z\alpha)r\ .$$

with

$$\sqrt{\alpha_1\alpha_2} = \sqrt{(mc^2-E)(mc^2+E)} = \sqrt{m^2c^4-E^2} = mc^2(Z\alpha)$$

$$\kappa = -(j+\frac{1}{2}) = -1 \qquad \text{since } j = 1/2.$$

$$s = \sqrt{\kappa^2-\gamma^2} = \sqrt{1-Z^2\alpha^2} \approx 1-\frac{1}{2}Z^2\alpha^2$$

Then the radial wave function of the ground state are given by

$$\begin{aligned} f(r) &= a_0\frac{\sqrt{\alpha_1\alpha_2}}{\rho}e^{-\rho}\rho^s \\ &= a_0\sqrt{\alpha_1\alpha_2}\,e^{-\rho}\rho^{s-1} \\ &= a_0 mc^2(Z\alpha)e^{-\rho}\rho^{-\frac{1}{2}Z^2\alpha^2} \\ &= A_0 e^{-\rho}\rho^{-\frac{1}{2}Z^2\alpha^2} \end{aligned}$$

and

$$
\begin{aligned}
g(r) &= b_0 \frac{\sqrt{\alpha_1\alpha_2}}{\rho} e^{-\rho}\rho^{s} \\
&= b_0 \sqrt{\alpha_1\alpha_2} e^{-\rho}\rho^{s-1} \\
&= b_0 mc^2 (Z\alpha) e^{-\rho}\rho^{-\frac{1}{2}Z^2\alpha^2} \\
&= -\frac{1}{2} a_0 mc^2 (Z\alpha)^2 e^{-\rho}\rho^{-\frac{1}{2}Z^2\alpha^2} \\
&= -\frac{1}{2}(Z\alpha) A_0 e^{-\rho}\rho^{-\frac{1}{2}Z^2\alpha^2}
\end{aligned}
$$

with

$$
A_0 = a_0(mc^2)Z\alpha\,, \qquad b_0 = -\frac{Z\alpha}{2}a_0
$$

The upper component *f*(*r*) is very similar to the non-relativistic wave function except for an enhanced (singular) part at small ρ which goes like $\rho^{-\frac{1}{2}Z^2\alpha^2}$. This singularity is very weak, and the solution is still integrable near the origin. The lower component g(r) is very much smaller (by a factor of $\frac{1}{2}Z\alpha$) than the upper component. Thus the relativistic solution differs from the non-relativistic solution only to the order of *Za*, or at very short distances.

((**Note**)) The radial function for the ground state in the non-relativistic theory

$$
R_{10} = \frac{2Z^{3/2}}{a^{3/2}} e^{-\frac{rZ}{a}} = 2(\frac{mc}{\hbar})^{3/2}(Z\alpha)^{3/2} e^{-\rho}
$$

with

$$
\rho = \frac{rZ}{a} = \frac{rZ}{\hbar^2} me^2 = r(Z\alpha)\frac{mc}{\hbar}
$$

where

$$
a = \frac{\hbar^2}{me^2} \text{ (Bohr radius)} \qquad ,
$$

$$
\frac{Z}{a} = \frac{mc}{\hbar} Z\alpha\,.
$$

44. Heisenberg's principle of uncertainty

In the Dirac theory,

$$H = c\boldsymbol{\alpha}\cdot\boldsymbol{p} + \beta mc^2 - \frac{Ze^2}{r}$$

From the Heisenberg's equation of motion, we get the relations,

$$\boldsymbol{\alpha} = \frac{1}{c}\boldsymbol{v}$$

$$\beta H + H\beta = 2mc^2$$

When

$$2\beta < H >= 2mc^2, \qquad \beta = \frac{mc^2}{E} = \frac{1}{\gamma} = \sqrt{1-\frac{v^2}{c^2}}$$

The Heisenberg's principle of uncertainty:

$$\Delta p_r \Delta r \approx \hbar$$

((**Special relativity**))

$$\boldsymbol{p} = \gamma m\boldsymbol{v}, \qquad E = \gamma mc^2 = c\sqrt{m^2c^2 + \boldsymbol{p}^2}$$

with

$$\gamma = \frac{1}{\sqrt{1-\frac{v^2}{c^2}}}$$

So we get the Hamiltonian

$$\begin{aligned} H &\approx \boldsymbol{v}\cdot\boldsymbol{p} + mc^2\frac{1}{\gamma} - \frac{Ze^2}{r} \\ &= \gamma mv^2 + mc^2\frac{1}{\gamma} - \frac{Ze^2}{r} \\ &= c\sqrt{\boldsymbol{p}^2 + m^2c^2} - \frac{Ze^2}{r} \end{aligned}$$

Note that

$$\boldsymbol{v}\cdot\boldsymbol{p}+mc^2\frac{1}{\gamma}=\boldsymbol{v}\cdot\gamma m\boldsymbol{v}+mc^2\frac{1}{\gamma}$$

$$=\frac{mv^2}{\sqrt{1-\frac{v^2}{c^2}}}+mc^2\sqrt{1-\frac{v^2}{c^2}}$$

$$=\frac{mc^2}{\sqrt{1-\frac{v^2}{c^2}}}$$

$$=\sqrt{m^2c+cp}$$

We now consider the Hamiltonian given by

$$H=c\sqrt{(\Delta p_r)^2+m^2c^2}-\frac{Ze^2}{\hbar}\Delta p_r$$

We take a derivative of H with respect to Δp_r

$$\frac{\partial}{\partial(\Delta p_r)}H=\frac{c\Delta p_r}{\sqrt{(\Delta p_r)^2+m^2c^2}}-\frac{Ze^2}{\hbar}=0$$

Then we get

$$\frac{c\Delta p_r}{\sqrt{(\Delta p_r)^2+m^2c^2}}=\frac{Ze^2}{\hbar}$$

or

$$\frac{(\Delta p_r)^2}{(\Delta p_r)^2+m^2c^2}=(Z\alpha)^2$$

From this, $(\Delta p_r)^2$ can be obtained as

$$(\Delta p_r)^2=m^2c^2\frac{(Z\alpha)^2}{1-(Z\alpha)^2}$$

or

$$\Delta p_r = \frac{mcZ\alpha}{\sqrt{1-(Z\alpha)^2}}$$

From the relation $\Delta p_r \Delta r \approx \hbar$ we get

$$\Delta r \approx \frac{\hbar}{\Delta p_r} = \frac{\hbar}{mcZ\alpha}\sqrt{1-(Z\alpha)^2} \approx \frac{\hbar}{mcZ\alpha}$$

Then the local minimum of H is given by

$$H = mc^2\sqrt{1-(Z\alpha)^2}$$

which is exactly the same as the value of E_{ground} in the relativistic theory.

45. Determination of C_q (a_q, b_q)

We derive the recursion relation for C_q fro the relation

$$(s+q-\kappa)a_q + \gamma b_q = a_{q-1} + \mu b_{q-1}$$

$$C_q = \frac{a_q}{s+q+\kappa-\dfrac{\gamma}{\mu}} = \frac{b_q}{\dfrac{1}{\mu}(s+q-\kappa)+\gamma}$$

From these equations we get

$$C_q = \frac{\gamma(\mu-\dfrac{1}{\mu})+2(s+q-1)}{q(2s+q)}C_{q-1}$$

where

For $q = n_r+1$, $C_q = 0$. Then we have

$$\gamma(\mu-\frac{1}{\mu})+2(s+n_r)=0$$

Finally we get the recursion formula,

$$C_q = \frac{2(s+q-1)-2(s+n_r)}{q(q+2s)} C_{q-1}$$
$$= \frac{2(q-1-n_r)}{q(q+2s)} C_{q-1}$$

For $q = 1$,

$$C_1 = \frac{2(-n_r)}{1(1+2s)} C_0 ,$$

For $q = 2$,

$$C_2 = \frac{2(1-n_r)}{2(2+2s)} C_1$$
$$= \frac{2(1-n_r)}{2(2+2s)} \frac{2(-n_r)}{1(1+2s)} C_0$$
$$= \frac{2^2(-1)^2 n_r(n_r-1)}{2!(1+2s)(2+2s)} C_0$$

For $q = 3$,

$$C_3 = \frac{2(2-n_r)}{3(3+2s)} C_2$$
$$= \frac{2^3(-1)^3 n_r(n_r-1)(n_r-2)}{3!(1+2s)(2+2s)(3+2s)} C_0$$

In general

$$C_k = \frac{2^k(-1)^k[n_r!/(n_r-k)!]}{k!(1+2s)(2+2s)...(k+2s)} C_0$$

where

$$C_q = \frac{a_q}{s+q+\kappa-\frac{\gamma}{\mu}} = \frac{b_q}{\frac{1}{\mu}(s+q-\kappa)+\gamma}$$

REFERENCES

E. Fermi, Notes on Quantum Mechanics (The University of Chicago Press, 1961).

J.D. Bjorken and S.D. Drell, Relativistic Quantum Mechanics (McGraw-Hill, New York, 1964)
J.J. Sakurai, Advanced Quantum Mechanics (Addison-Wesley, New York, 1967).
M.E. Rose, Relativistic Electron Theory (John Wiley & Sons, New York, 1961).
A. Das, Lectures on Quantum mechanics, second edition (World Scientific, 2012).
F.J, Dyson, Advanced Quantum Mechanics (World Scientific, 2007).
S.S. Schweber, An Introduction to Relativistic Quantum Field Theory (Row, Peterson, 1961).
F. Schwabl, Advanced *Quantum Mechanics* (Springer Verlag, Berlin, 2005).
F. Gross, Relativistic Quantum Mechanics and Field Theory (Wiley-VCH, 1993).
Eugen Merzbacher, *Quantum Mechanics*, third edition (John Wiley & Sons, New York, 1998).
Ramamurti Shankar, *Principles of Quantum Mechanics*, second edition (Springer, New York, 1994).
Leonard Schiff, *Quantum Mechanics* (McGraw-Hill Book Company, Inc, New York, 1955).
B.R. Holstein, Topics in ADVANCED Quantum Mechanics (Addison-Wesley, 1992).
H. Bethe and E.E. Salpeter, Quantum Mechanics of one and two-electron atoms

---

APPENDIX-1

Commutation relations

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

$$I_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

Using the Kronecker product, the matrices α_1, α_2, α_3, and β are given by

$$\alpha_1 = \sigma_1 \otimes \sigma_1 = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & \sigma_1 \\ \sigma_1 & 0 \end{pmatrix}$$

$$\alpha_2 = \sigma_2 \otimes \sigma_2 = \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & \sigma_2 \\ \sigma_2 & 0 \end{pmatrix}$$

$$\alpha_3 = \sigma_3 \otimes \sigma_3 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & \sigma_3 \\ \sigma_3 & 0 \end{pmatrix}$$

$$\beta = \sigma_z \otimes I_2 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} = \begin{pmatrix} I_2 & 0 \\ 0 & -I_2 \end{pmatrix}$$

$$\gamma_1 = -i\beta\alpha_1 = \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & -i & 0 \\ 0 & i & 0 & 0 \\ i & 0 & 0 & 0 \end{pmatrix},$$

$$\gamma_2 = -i\beta\alpha_2 = \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}$$

$$\gamma_3 = -i\beta\alpha_3 = \begin{pmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & i \\ i & 0 & 0 & 0 \\ 0 & -i & 0 & 0 \end{pmatrix}$$

$$\beta = \gamma_4 = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}$$

$$\Sigma_k = \begin{pmatrix} \sigma_k & 0 \\ 0 & \sigma_k \end{pmatrix}$$

$$\Sigma_1 = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}, \qquad \Sigma_2 = \begin{pmatrix} 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \end{pmatrix}$$

$$\Sigma_3 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix},$$

$$\gamma_5 = \begin{pmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \\ -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}$$

$$\alpha_k = i\gamma_4\gamma_k = \begin{pmatrix} 0 & \sigma_k \\ \sigma_k & 0 \end{pmatrix}$$

$$\gamma_4\gamma_k = -\gamma_k\gamma_4$$

$$\{\alpha_i, \alpha_j\} = 2\delta_{ij} I \,,$$

$$\{\alpha_i, \beta\} = 0 \,, \qquad \beta^2 = I$$

$$\alpha_k = -\Sigma_k\gamma_5 = -\gamma_5\Sigma_k \,,$$

$$[\beta, \Sigma_k] = 0$$

$$\beta = \gamma_4$$

$$\gamma_5 = \gamma_1\gamma_2\gamma_3\gamma_4 \,,$$

$$\Sigma_k = -i\gamma_i\gamma_j \qquad (i, j, k\text{: cyclic})$$

$$[\gamma_5, \Sigma_k] = 0 \,,$$

$$[\gamma_5, \alpha_k] = 0 \,,$$

$$[\gamma_4, \Sigma_k] = 0$$

$$[\Sigma_i, \Sigma_j] = 2i\Sigma_k, \qquad \Sigma_i\Sigma_j = -\Sigma_j\Sigma_i = i\Sigma_k \qquad (i, j, \text{ and } k; \text{ cyclic})$$

$$[\gamma_5\Sigma_k, \Sigma_j] = \gamma_5\Sigma_k\Sigma_j - \Sigma_j\gamma_5\Sigma_k = \gamma_5[\Sigma_k, \Sigma_j].$$

$$\{\gamma_5, \beta\} = 0.$$

$$\gamma_1^T = -\gamma_1, \qquad \gamma_2^T = \gamma_2, \qquad \gamma_3^T = -\gamma_3, \qquad \gamma_4^T = \gamma_4$$

The helicity operator

$$\boldsymbol{\Sigma} \cdot \hat{\boldsymbol{p}}$$

For two arbitrary vectors $\boldsymbol{A}$ and $\boldsymbol{B}$,

$$(\hat{\boldsymbol{\sigma}} \cdot \boldsymbol{A})(\hat{\boldsymbol{\sigma}} \cdot \boldsymbol{B}) = (\boldsymbol{A} \cdot \boldsymbol{B})\hat{1} + i\hat{\boldsymbol{\sigma}} \cdot (\boldsymbol{A} \times \boldsymbol{B})$$

where

$$\boldsymbol{A} = (A_x, A_y, A_z) \text{ and } \quad \boldsymbol{B} = (B_x, B_y, B_z)$$

$$\boldsymbol{J} = \boldsymbol{L} + \frac{\hbar}{2}\boldsymbol{\Sigma} = \begin{pmatrix} \boldsymbol{L} + \frac{\hbar}{2}\boldsymbol{\sigma} & 0 \\ 0 & \boldsymbol{L} + \frac{\hbar}{2}\boldsymbol{\sigma} \end{pmatrix}$$

((**Mathematica**))

```
Clear["Global`*"];
exp_* := exp /. {Complex[re_, im_] :> Complex[re, -im]};
σx = (0 1
      1 0); σy = (0 -i
                  i  0); σz = (1  0
                               0 -1);
I2 = IdentityMatrix[2]; I4 = IdentityMatrix[4];
α1 = KroneckerProduct[σx, σx]; α2 = KroneckerProduct[σx, σy];
α3 = KroneckerProduct[σx, σz]; β = KroneckerProduct[σz, I2];
γ1 = -i β.α1 // Simplify; γ2 = -i β.α2 // Simplify; γ3 = -i β.α3 // Simplify; γ4 = β;
γ5 = γ1.γ2.γ3.γ4;

Σ1 = KroneckerProduct[I2, σx]; Σ2 = KroneckerProduct[I2, σy];
Σ3 = KroneckerProduct[I2, σz];

Σ1 // MatrixForm
```

$$\begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

```
Σ2 // MatrixForm
```

$$\begin{pmatrix} 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \end{pmatrix}$$

```
Σ3 // MatrixForm
```

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

```
Σ1.Σ1 // Simplify
{{1, 0, 0, 0}, {0, 1, 0, 0}, {0, 0, 1, 0}, {0, 0, 0, 1}}

Σ1 + ⅈ γ2. γ3 // Simplify
{{0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}}

Σ1.Σ1 + Σ2.Σ2 + Σ3.Σ3 - 3 I4
{{0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}}

Σ1.Σ2 - Σ2.Σ1 - 2 ⅈ Σ3
{{0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}}

α1.Σ1 - Σ1.α1
{{0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}}

α1 + ⅈ γ1.γ4
{{0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}}

α1 +  Σ1.γ5
{{0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}}

α1 + γ5. Σ1
{{0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}}

α1.β + β.α1
{{0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}}
```

```
β.Σ1 - Σ1.β
{{0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}}

γ5 .Σ1 - Σ1.γ5
{{0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}}

α1 .Σ1 - Σ1.α1
{{0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}}

γ5 .β + β.γ5
{{0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}}

γ5.γ5
{{1, 0, 0, 0}, {0, 1, 0, 0}, {0, 0, 1, 0}, {0, 0, 0, 1}}

α1 .α2 +  α2.α1
{{0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}}

α1 .α1
{{1, 0, 0, 0}, {0, 1, 0, 0}, {0, 0, 1, 0}, {0, 0, 0, 1}}

γ4.Σ1 - Σ1.γ4
{{0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}}

γ1.γ2 + γ2.γ1
{{0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}}

Transpose[γ1] + γ1
{{0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}}

γ5 .α1 - α1.γ5
{{0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}}

γ4 .γ1 + γ1.γ4
{{0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}, {0, 0, 0, 0}}
```

APPENDIX II
Klein-Gordon equation
((Problem))
The relativistic wave equation for bosons of rest mass *m* may be obtained by the relation

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

through the identifications

$$E \rightarrow i\hbar\frac{\partial}{\partial t}, \qquad \boldsymbol{p} \rightarrow \frac{\hbar}{i}\nabla$$

(a) Obtain the wave equation relevant to bosons of rest mass *m*. This equation is called the <u>Klein-Gordon equation</u>.

(b) What form does this equation assume for photons?

(c) Suppose that the wavefunction is independent of time *t*. It depends only on *r*. Using the spherical co-ordinates; $\{r, \theta, \phi\}$, find the differential equation for the wavefunction $\psi(r)$. Show that $\psi(r)$ has the form of $\psi(r) = A\frac{e^{-r/a}}{r}$, where *A* and *a* are constants. <u>We assume that *l* = 0.</u>

(d) Find the expression for the characteristic length *a*.

(e) Use this equation to show that there is a local conservation law of the form

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \boldsymbol{j} = 0$$

with

$$\boldsymbol{j} = \frac{\hbar}{2mi}(\psi^*\nabla\psi - \psi\nabla\psi^*).$$

Determine the form of $\rho(\boldsymbol{r}, t)$. From this form for ρ, give an argument for why the Klein-Gordon equation is not a good candidate for a one-particle relativistic wave equation in plane of the Schrodinger equation, for which $\rho = \psi^*\psi$

((**Solution**))

(a)

We start with

$$E^2\psi = (\boldsymbol{p}^2c^2 + m^2c^4)\psi,$$

with

$$E \rightarrow i\hbar\frac{\partial}{\partial t}, \qquad \boldsymbol{p} \rightarrow \frac{\hbar}{i}\nabla$$

Then we have

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

or

$$\nabla^2 \psi - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\psi = \frac{m^2 c^2}{\hbar^2}\psi \qquad \text{(Klein-Gordon equation)}$$

(b) For photon, the mass m is equal to zero. Then we have the wave equation as

$$\nabla^2 \psi - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\psi = 0$$

(c) Suppose that the wavefunction is independent of time t. It depends only on r.

$$\frac{1}{r}\frac{\partial}{\partial r}(\frac{\partial}{\partial r} r)\psi(r) = \frac{m^2 c^2}{\hbar^2}\psi$$

We assume that $\psi = \frac{u}{r}$.

$$\frac{d^2}{dr^2}u(r) = \frac{m^2 c^2}{\hbar^2}u(r) = \frac{1}{a^2}u(r).$$

Then we have the

$$u = Ae^{-r/a}$$

or

$$\psi = A\frac{e^{-r/a}}{r}$$

(d)

a is the characteristic length and is defined by

$$a = \frac{\hbar}{mc}.$$

(e) The current density is given by

$$\boldsymbol{j} = \frac{\hbar}{2mi}(\psi^*\nabla\psi - \psi\nabla\psi^*)$$

$$\begin{aligned}
\nabla\cdot\boldsymbol{j} &= \frac{\hbar}{2mi}[\nabla\cdot(\psi^*\nabla\psi) - \nabla\cdot(\psi\nabla\psi^*)] \\
&= \frac{\hbar}{2mi}(\nabla\psi^*\cdot\nabla\psi + \psi^*\nabla^2\psi - \nabla\psi\nabla\psi^* - \psi\nabla^2\psi^*) \\
&= \frac{\hbar}{2mi}(\psi^*\nabla^2\psi - \psi\nabla^2\psi^*)
\end{aligned}$$

Using the equation of continuity, we have

$$\frac{\partial\rho}{\partial t} = -\nabla\cdot\boldsymbol{j} = -\frac{\hbar}{2mi}(\psi^*\nabla^2\psi - \psi\nabla^2\psi^*)$$

We use the Klein-Gordon equation

$$\nabla^2\psi = \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\psi + \frac{m^2c^2}{\hbar^2}\psi, \qquad \nabla^2\psi^* = \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\psi^* + \frac{m^2c^2}{\hbar^2}\psi^*$$

Then we get

$$\begin{aligned}
\frac{\partial\rho}{\partial t} &= -\frac{\hbar}{2mi}[\psi^*(\frac{1}{c^2}\frac{\partial^2}{\partial t^2}\psi + \frac{m^2c^2}{\hbar^2}\psi) - \psi(\frac{1}{c^2}\frac{\partial^2}{\partial t^2}\psi^* + \frac{m^2c^2}{\hbar^2}\psi^*)] \\
&= -\frac{\hbar}{2mc^2i}(\psi^*\frac{\partial^2}{\partial t^2}\psi - \psi\frac{\partial^2}{\partial t^2}\psi^*) \\
&= -\frac{\hbar}{2mc^2i}\frac{\partial}{\partial t}(\psi^*\frac{\partial}{\partial t}\psi - \psi\frac{\partial}{\partial t}\psi^*)
\end{aligned}$$

Thus we have

$$\boxed{\rho = \frac{i\hbar}{2mc^2}(\psi^*\frac{\partial}{\partial t}\psi - \psi\frac{\partial}{\partial t}\psi^*)}$$

Suppose that

$$\psi^*\frac{\partial}{\partial t}\psi = \alpha + i\beta$$

where α and β are real. Then we have

$$\psi \frac{\partial}{\partial t}\psi^* = \alpha - i\beta$$

Then we have

$$\rho = \frac{i\hbar}{2mc^2}[\alpha + i\beta - (\alpha - i\beta)] = \frac{i\hbar}{2mc^2}2i\beta = -\frac{\beta\hbar}{mc^2}$$

When $\beta > 0$, the probability density could be negative, which is inconsistent with the requirement that ρ should be positive. In this sense, the Klein-Gordon equation is not a good candidate for a one-particle relativistic wave equation in plane of the Schrodinger equation, for which $\rho = \psi^* \psi$