5° Discrete symmetries of the Dirac equation

Goals:
- Identify symmetries that facilitate the solution of the relativistic Coulomb problem.
- Gain further insight into the physical meaning of the internal degrees of freedom associated with the Dirac spinor.

Notation: Here and in the following we use "natural units" where $\hbar = c = 1$. The Dirac Hamiltonian then reads

$$H = \vec{\alpha}\cdot\vec{p} + \beta m + V(\vec{r})$$

a) **Parity**: The parity transformation (= space inversion)

$$\vec{r} \to -\vec{r}$$

transforms a right-handed coordinate system into a left-handed one. In non-relativistic quantum mechanics the parity operator $\tilde{P}$ acts on wave functions as

$$\tilde{P}\psi(\vec{r}) = \psi(-\vec{r})$$

Because $\tilde{P}^2 = \mathbb{1}$, the eigenvalues of $\tilde{P}$ are ± 1:

$$\left.\begin{array}{ll} \psi(-\vec{r}) = \psi(\vec{r}) & \text{even} \\ \psi(-\vec{r}) = -\psi(\vec{r}) & \text{odd} \end{array}\right\} \text{parity state}$$

More generally $\tilde{P} : |\psi\rangle \to \tilde{P}|\psi\rangle$

and we require that

$$\langle\psi|\tilde{P}^{+}\vec{r}\,\tilde{P}|\psi\rangle = -\langle\psi|\vec{r}|\psi\rangle$$

for any $|\psi\rangle$, which implies

$$\tilde{P}^{+}\vec{r}\,\tilde{P} = -\vec{r} \Rightarrow \vec{r}\,\tilde{P} = -\tilde{P}\,\vec{r}$$

using the fact that $\tilde{P}$ is unitarity.

Thus $\vec{r}$ is odd under parity. Because $\vec{p} = -i\nabla_r$ describes spatial translations, likewise

$$\vec{p}\,\tilde{P} = -\tilde{P}\,\vec{p} \Rightarrow \vec{p} \text{ is odd}$$

On the other hand, for inversion-symmetric potentials with $V(-\vec{r}) = V(\vec{r})$ we expect H to be even. Because H is linear in $\vec{p}$, this requires a nontrivial action in spinor space. We therefore define

$$P = \tilde{P}\,U_p \qquad \left.\begin{array}{l}\tilde{P} : \text{space inversion} \\ U_p : \text{unitary } 4\times4 \text{ matrix}\end{array}\right\}$$

and require

$$P^{+} H P = U_p^{+} \underbrace{\tilde{P}^{+}(\vec{\alpha}\cdot\vec{p})\,\tilde{P}}_{-(\vec{\alpha}\cdot\vec{p})} U_p \; +$$

$$+ U_P^\dagger \underbrace{\tilde{P}^\dagger \beta m \tilde{P}}_{=\beta m} U_P + U_P^\dagger \underbrace{\tilde{P}^\dagger V(\vec{r}) \tilde{P}}_{V(-\vec{r}) = V(\vec{r})} U_P$$

$$= -\left(U_P^\dagger \vec{\alpha}\, U_P\right)\cdot \vec{p} + \left(U_P^\dagger \beta U_P\right) m + \underbrace{U_P^\dagger U_P}_{U_P^2} V(\vec{r})$$

$$\overset{!}{=} H$$

$$\Rightarrow \quad \underline{U_P^\dagger \vec{\alpha}\, U_P = -\vec{\alpha}, \quad U_P^\dagger \beta U_P = \beta, \quad U_P^2 = \mathbb{1}}$$

Since the α^k anticommute with β,

$$\alpha^k \beta = -\beta \alpha^k \quad \Rightarrow \quad \alpha^k = -\beta \alpha_k \beta$$

we can choose $\underline{U_P = \beta}$ and identify the parity operator as

$$\underline{P = \tilde{P} \beta}$$

A spinor state is an eigenstate of P if

$$\psi(\vec{r}) = \begin{pmatrix} \psi_1(\vec{r}) \\ \psi_2(\vec{r}) \\ \psi_3(\vec{r}) \\ \psi_4(\vec{r}) \end{pmatrix} = \pm \beta \psi(-\vec{r}) = \pm \begin{pmatrix} \psi_1(-\vec{r}) \\ \psi_2(-\vec{r}) \\ -\psi_3(-\vec{r}) \\ -\psi_4(-\vec{r}) \end{pmatrix}$$

Upper and lower components of the Dirac spinor have <u>opposite parity</u>.

b) Charge conjugation

We look for a transformation that transforms particle solutions into antiparticle solutions. The latter satisfy the Dirac equation with opposite charge. In covariant notation and in the presence of a electromagnetic field

$$A_\mu = (\Phi, -\vec{A})$$

the equations are

P $$(i\gamma^\mu \partial_\mu - e\gamma^\mu A_\mu - m)\psi = 0 \qquad \text{particle}$$

$$\Big\downarrow C$$

AP $$(i\gamma^\mu \partial_\mu + e\gamma^\mu A_\mu - m)\psi = 0 \qquad \text{antiparticle}$$

Taking the complex conjugate of P yields

$$(-i(\gamma^\mu)^* \partial_\mu - e(\gamma^\mu)^* A_\mu - m)\psi^* = 0$$

If we can find a 4×4 matrix $\tilde{C}$ such that

$$\tilde{C}(\gamma^\mu)^* \tilde{C}^{-1} = -\gamma^\mu$$

then the state $C\psi := \tilde{C}\psi^*$ satisfies

$$0 = \tilde{C}(-i(\gamma^\mu)^* \partial_\mu - e(\gamma^\mu)^* A_\mu - m)\tilde{C}^{-1}\underbrace{\tilde{C}\psi^*}_{= C\psi}$$

$$= (i\gamma^\mu \partial_\mu + e\gamma^\mu A_\mu - m)C\psi \iff \text{AP}$$

To identify $\tilde{C}$, recall that

$$\gamma^0 = \beta \,, \quad \gamma^k = \beta \alpha^k \,, \quad k = 1,2,3$$

where α^1, α^3 are real and α^2 imaginary. Moreover $\{\gamma^\mu, \gamma^\nu\} = 2 g^{\mu\nu} \mathbb{1}$. If we set

$$\tilde{C} = i \gamma^2$$

it follows that

$$(\tilde{C})^2 = -(\gamma^2)^2 = \mathbb{1} \quad \Rightarrow \quad \tilde{C}^{-1} = \tilde{C}$$

$$\tilde{C} (\gamma^\mu)^* \tilde{C}^{-1} = i \gamma^2 \gamma^\mu i \gamma^2 = \qquad (\mu \neq 2)$$

$$= - \gamma^2 \gamma^\mu \gamma^2 = (\gamma^2)^2 \gamma^\mu = - \gamma^\mu$$

and $\tilde{C} (\gamma^2)^* \tilde{C}^{-1} = - \gamma^2 \underbrace{(\gamma^2)^*}_{-\gamma^2} \gamma^2 = (\gamma^2)^2 \gamma^2 = - \gamma^2$

$\Rightarrow$ charge conjugation can be realized by

$$C : \psi \rightarrow \tilde{C} \psi^* = i \gamma^2 \psi^*$$

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c) Time reversal

Recall: A dynamical problem is time-reversal invariant if, given a solution $X(t)$, the time-reversed trajectory $X(-t)$ is also a solution.

Examples: • Newtonian mechanics

$$m \frac{d^2\vec{r}}{dt^2} = \vec{F}(\vec{r})$$

is time-reversal invariant because the LHS is a second order derivative. This property is spoiled by velocity-dependent forces (e.g. friction or magnetic fields)

• The non-relativistic Schrödinger equation

$$i\,\partial_t \psi = H\psi$$

is first order in time and hence not time-reversal invariant. However, if H is real, time reversal $t \to -t$ is equivalent to complex conjugation:

$$-i\,\partial_t \psi^* = i\,\partial_{-t}\psi^* = H\psi^*$$

$\Rightarrow$ ψ^* is the time-reversed solution.

• For the Dirac equation this does not work because the α^k cannot all be real.

We therefore make the ansatz

$$T = U_T K$$

for the time-reversal operator, where K is complex conjugation and U_T is unitary.

We start from the Dirac equation

$$i\partial_t \psi = H\psi \qquad \text{D}$$

with $H = \vec{\alpha}\cdot\vec{p} + \beta m = -i\vec{\alpha}\cdot\nabla + \beta m$

and express $\alpha^k = \gamma^0\gamma^k$, $\beta = \gamma^0$.

Application of T to the LHS of D yields

$$\underline{T\, i\partial_t \psi} = T\, i\partial_t (T^{-1}T)\psi =$$

$$= U_T K\, i\partial_t\, K U_T^{-1} U_T K \psi =$$

$$= U_T(-i\partial_t)\psi^* = i\partial_{-t}(U_T\psi^*) = \underline{i\partial_{-t}(T\psi)}$$

as in the Schrödinger case. Now U_T has to be chosen such that the RHS of D remains invariant. This requires

$$TH\psi = \underline{THT^{-1}}(T\psi) \overset{!}{=} \underline{H}(T\psi)$$

$$\Rightarrow \begin{cases} T(i\gamma^0\gamma^k)T^{-1} = i\gamma^0\gamma^k, & k = 1,2,3 \\ T\gamma^0 T^{-1} = \gamma^0 \end{cases}$$

The complex conjugation K induces a sign change for $k = 1,2,3$ but not for γ^0:

$$\begin{cases} U_T^{-1}\gamma^k U_T = -(\gamma^k)^* & k = 1,2,3 \\ U_T^{-1}\gamma^0 U_T = \gamma_0^* \end{cases}$$

In the standard representation $\gamma^0, \gamma^1, \gamma^3$ are real and γ^2 is imaginary. We therefore set

$$U_T = \gamma^1 \gamma^3 \,, \quad U_T^{-1} = \gamma^3 \gamma^1$$

$$\Rightarrow \quad U_T^{-1} \gamma^1 U_T = \gamma^3 (\gamma^1)^2 \gamma^1 \gamma^3 = - \gamma^3 \gamma^1 \gamma^3 =$$

$$= \gamma^1 (\gamma^3)^2 = - \gamma^1 = - (\gamma^1)^*$$

$$U_T^{-1} \gamma^2 U_T = \gamma^3 \gamma^1 \gamma^2 \gamma^1 \gamma^3 = \gamma^2 \big(\underbrace{\gamma^3 (\gamma^1) \gamma^3}_{=1} \big)$$

$$= \gamma^2 = - (\gamma^2)^*$$

$$U_T^{-1} \gamma^0 U_T = \gamma^0$$

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d) CPT invariance

In summary, we have found the following representations of the three discrete symmetries:

$$\left. \begin{aligned} P: &\quad \psi(\vec{r}, t) \longrightarrow \gamma^0 \psi(-\vec{r}, t) \\ C: &\quad \psi(\vec{r}, t) \longrightarrow i \gamma^2 \big(\psi(\vec{r}, t)^* \big) \\ T: &\quad \psi(\vec{r}, t) \longrightarrow \gamma^1 \gamma^2 \big(\psi(\vec{r}, t)^* \big) \end{aligned} \right\}$$

Combining all three yields

$$(CPT)\, \psi(\vec{r}, t) = \underbrace{i \, \gamma^0 \gamma^1 \gamma^2 \gamma^3}_{=:\, \gamma^5} \psi(-\vec{r}, t)$$

with $\gamma^5 = \begin{pmatrix} 0 & \mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix}$ in the standard representation. Exercise

<u>Remark:</u> Although individual symmetries can be broken e.g. by the weak interaction, any Lorentz-invariant quantum field theory is also CPT-invariant.

6° The relativistic Coulomb problem

<u>Goal:</u> To solve the stationary Dirac equation

$$H\psi(\vec{r}) = (\vec{\alpha}\vec{p} + \beta m + V(\vec{r}))\psi(\vec{r}) = E\psi(\vec{r})$$

for radially symmetric $V(\vec{r})$, specifically $V = -\frac{Ze^2}{r}$

Because of the symmetry of the potential, the eigenfunctions can be chosen to be eigenfunctions of parity and total angular momentum.

Parity invariance implies

$$\psi(\vec{r}) = \begin{pmatrix} \varphi(\vec{r}) \\ \chi(\vec{r}) \end{pmatrix} \overset{!}{=} \pm \begin{pmatrix} \varphi(-\vec{r}) \\ -\chi(-\vec{r}) \end{pmatrix}$$

where φ, χ are 2-spinors.

We start by constructing the angular momentum eigenstates.

a) Eigenfunctions of total angular momentum

The total angular momentum is $\vec{J} = \vec{L} + \vec{S}$ with $\vec{L} = \vec{r} \times \vec{p}$ and $\vec{S} = \frac{1}{2} \vec{\Sigma}$.

We need joint eigenstates of $\vec{J}^2$ and J_z with quantum numbers j and $m := m_j$. These are constructed as superpositions of the product states

$$\left.\begin{aligned} \underbrace{|\, l, m - \tfrac{1}{2} \rangle}_{\text{orbital}} \underbrace{|\uparrow\rangle}_{\text{spin}} &= \underbrace{Y_l^{m-\frac{1}{2}}(\theta, \phi)}_{\text{spherical harmonics}} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ |\, l, m + \tfrac{1}{2} \rangle |\downarrow\rangle &= Y_l^{m+\frac{1}{2}}(\theta, \phi) \begin{pmatrix} 0 \\ 1 \end{pmatrix} \end{aligned}\right\}$$

The z-components add up as

$$m = m_j = m_l + m_s = m_l \pm \frac{1}{2}$$

and the possible values of j are

$$\left.\begin{aligned} j &= l \pm \frac{1}{2} & l &= 1, 2, 3 \\ j &= \frac{1}{2} & l &= 0 \end{aligned}\right\}$$

The appropriate linear combinations are the spin-angular functions defined by

$$\mathcal{Y}_\ell^{j=\ell\pm\frac{1}{2},m} = \frac{1}{\sqrt{2\ell+1}} \begin{pmatrix} \pm\sqrt{\ell \pm m + \frac{1}{2}} \cdot Y_\ell^{m-\frac{1}{2}}(\theta,\phi) \\ \sqrt{\ell \mp m + \frac{1}{2}} \cdot Y_\ell^{m+\frac{1}{2}}(\theta,\phi) \end{pmatrix}$$

Clebsch-Gordan coefficients

These are joint eigenstates of $\vec{J}^2$, J_z and $\vec{L}^2$ but not of L_z.

We check the action of J_z:

$$J_z \mathcal{Y}_\ell^{j=\ell\pm\frac{1}{2},m} = \left(L_z + \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right) \mathcal{Y}_\ell^{j=\ell\pm\frac{1}{2},m} =$$

$$= \frac{1}{\sqrt{2\ell+1}} \begin{pmatrix} \pm\left(m - \frac{1}{2} + \frac{1}{2}\right)\sqrt{\ell \pm m + \frac{1}{2}}\; Y_\ell^{m-\frac{1}{2}} \\ \left(m + \frac{1}{2} - \frac{1}{2}\right)\sqrt{\ell \mp m + \frac{1}{2}}\; Y_\ell^{m+\frac{1}{2}} \end{pmatrix} = m\, \mathcal{Y}_\ell^{j=\ell\pm\frac{1}{2},m}$$

The parity of the spherical harmonics is determined by ℓ,

$$Y_\ell^m(-\vec{r}) = (-1)^\ell Y_\ell^m(\vec{r})$$

Thus the two possible values $\ell = j \pm \frac{1}{2}$ associated with a given j lead to states of opposite parity.

This leaves two possibilities for eigenstates of definite parity and angular momentum:

$$\psi_A(\vec{r}) = \begin{pmatrix} \varphi_A(\vec{r}) \\ \chi_A(\vec{r}) \end{pmatrix} = \begin{pmatrix} u_A(r)\, \mathcal{Y}^{j\mu}_{j-\frac{1}{2}}(\theta,\phi) \\ -i\, v_A(r)\, \mathcal{Y}^{j\mu}_{j+\frac{1}{2}}(\theta,\phi) \end{pmatrix}$$

$$\psi_B(\vec{r}) = \begin{pmatrix} \varphi_B(\vec{r}) \\ \chi_B(\vec{r}) \end{pmatrix} = \begin{pmatrix} u_B(r)\, \mathcal{Y}^{j\mu}_{j+\frac{1}{2}}(\theta,\phi) \\ -i\, v_B(r)\, \mathcal{Y}^{j\mu}_{j-\frac{1}{2}}(\theta,\phi) \end{pmatrix}$$

where $u_{A,B}(r)$ and $v_{A,B}(r)$ are radial wave functions.

Note that ψ_A, ψ_B are not eigenstates of $\vec{L}^2$.

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b) Derivation of the radial wave equations

Inserting the two-component ansatz into the Dirac equation yields

$$\left.\begin{aligned} (E - m - V(r))\,\varphi - (\vec{\sigma}\cdot\vec{p})\,\chi &= 0 \\ (E + m - V(r))\,\chi - (\vec{\sigma}\cdot\vec{p})\,\varphi &= 0 \end{aligned}\right\}$$

To evaluate the kinetic energy terms we use

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

For vectors $\vec{a}$ with commuting coefficients