Chapter 5

Dirac Equation with Interactions

5.1 Dirac Hamiltonian

Originally Dirac postulated a linear equation with a standard Hamiltonian form:

$$i \, \frac{\partial \psi}{\partial t} \, (\vec{x}, t) \; = \; H_0 \; \psi(\vec{x}, t) \; . \tag{5.1}$$

This proposed equation is consistent with the requirements that in a relativistic theory there is a wave function that can be determined by an equation of first order in the time derivative so that the probability will be independent of time. The theory also should be canonical and contain a Hamiltonian H_0 so that the wave equation and quantization rules are conventional. In order for (5.1) to be Lorentz covariant, the most general H_0 must also be first order in the space derivatives:

$$H_0 \; = \; \frac{1}{i} \left[\alpha_1 \, \frac{\partial}{\partial x^1} \; + \; \alpha_2 \, \frac{\partial}{\partial x^2} \; + \; \alpha_3 \, \frac{\partial}{\partial x^3} \right] \; + \beta m \; . \tag{5.2}$$

Here α_i and β are assumed to be dimensionless constants, independent of space and time, that commute with $\vec{r}$ and $\vec{p}$ (guarantees translational invariance). Defining

$$\vec{\alpha} \; = \; (\alpha_1, \; \alpha_2, \; \alpha_3) \tag{5.3}$$

and using $\vec{p} = \frac{\vec{\nabla}}{i}$, the Hamiltonian form of the Dirac equation is given by

$$i \frac{\partial \psi}{\partial t} = H_0 \, \psi(\vec{x}, t) \; . \tag{5.4}$$

This looks like the Schrödinger equation, however, the Dirac Hamiltonian

$$H_1 = \vec{\alpha} \cdot \vec{p} + \beta m \tag{5.5}$$

has quite a different structure.

The major constraints on $\vec{\alpha}$ and β arise from requiring the operator form of $E^2 = p^2 + m^2$ (i.e., the Klein-Gordon equation) still to be valid when acting on ψ. To systematically impose this requirement, we take the time derivative of (5.4),

$$\begin{aligned} i \frac{\partial^2 \psi}{\partial t^2} &= (\vec{\alpha} \cdot \vec{p} + \beta m) \frac{\partial \psi}{\partial t} \\ &= (\vec{\alpha} \cdot \vec{p} + \beta m) \left(\alpha \cdot \frac{\vec{p}}{i} \psi + \frac{\beta}{i} m \, \psi\right) \\ &= \left(\sum_k \frac{\alpha_k}{i} \frac{\partial}{\partial x^k} + \beta m\right) \left(\sum_j \frac{\alpha_j}{i^2} \frac{\partial}{\partial x^j} + \frac{\beta m}{i}\right) \psi \\ &= i \sum_{k,j} \frac{\alpha_j \alpha_k + \alpha_k \alpha_j}{2} \frac{\partial^2 \psi}{\partial x^k \partial x^j} - m \sum_k (\alpha_k \beta + \beta \alpha_k) \frac{\partial \psi}{\partial x^k} - i \beta^2 m^2 \, \psi \; . \end{aligned} \tag{5.6}$$

The left-hand side of (5.7) corresponds to the left-hand side of the Klein-Gordon equation operating on ψ (each component thereof). In order for the right-hand side of (5.7) to be equivalent to the Klein-Gordon equation for each component of ψ, the following anticommutation relations have to be valid

$$\begin{aligned} \{\alpha_k, \; \alpha_j\} &= 2\delta k_j \\ \{\alpha_k, \; \beta\} &= 0 \end{aligned} \tag{5.7}$$

From (5.8) follows that $\alpha_i^2 = \beta^2 = 1$.

As already shown in Chapter 6, the wave function has to have four components, $\psi = (\psi_1, \; \psi_2, \; \psi_3, \; \psi_4)$. The matrices $\vec{\alpha}$ and β are given by

$$\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix} \quad ; \quad \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} , \tag{5.8}$$

and $\vec{\alpha}$ and β are traceless.

5.2 Central-Force Problem

Here we want to solve the Dirac equation with a potential. A simplification is the consideration of a central potential $V(r)$. Then Hamiltonian takes the general form

$$H = \vec{\alpha} \cdot \vec{p} + \beta m + V(r) , \tag{5.9}$$

and the general task is the solution of the eigenvalue problem

$$(H - E)\psi = 0 . \tag{5.10}$$

For ψ we choose the ansatz $\psi \equiv (\varphi, \chi)$, where φ, χ are again two-component functions. Inserting this into (5.9), (5.10) leads to

$$\left[\begin{pmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & 0 \end{pmatrix} \vec{p} + \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} m + \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} (V - E) \right] \begin{pmatrix} \varphi \\ \chi \end{pmatrix} = 0 , \tag{5.11}$$

which gives

$$\begin{pmatrix} V - E + m & \vec{\sigma} \cdot \vec{p} \\ \vec{\sigma} \cdot \vec{p} & V - E - m \end{pmatrix} \begin{pmatrix} \varphi \\ \chi \end{pmatrix} = 0 . \tag{5.12}$$

This leads to the coupled equations for φ and χ:

$$
\begin{aligned}
(V - E + m)\,\varphi \;+\; \vec{\sigma}\,\cdot\,\vec{p}\,\chi \;&=\; 0 \\
\vec{\sigma}\,\cdot\,\vec{p}\,\varphi \;+\; (V - E - m)\,\chi \;&=\; 0
\end{aligned}
\tag{5.13}
$$

from which one can express the small component χ as

$$
\chi \;=\; \frac{-1}{V - E - m}\,\vec{\sigma}\,\cdot\,\vec{p}\,\varphi\;. \tag{5.14}
$$

For a closer inspection, let us consider the action of the parity operator on the Dirac spinor ψ. For an arbitrary four-vector, one has under parity operations

$$
x' \;\equiv\; Px \;=\; (x_0,\; -\vec{x})\;. \tag{5.15}
$$

Thus

$$
\begin{aligned}
\psi'(x') \;&=\; \beta\,\psi(x) \\
\psi'(x_0,\; -\vec{x}) \;&=\; \beta\,\psi(x_0,\; \vec{x}) \\
\psi'(x_0,\; \vec{x}) \;&=\; \beta\,\psi(x_0,\; -\vec{x})\;.
\end{aligned}
\tag{5.16}
$$

Define $P \;\equiv\; P_0\beta$ with

$$
P_0\;\psi(t,\;\vec{x}) \;=\; \psi(t,\;-\vec{x}) \tag{5.17}
$$

and

$$
P_0\,\vec{\sigma}\,\cdot\,\vec{p} \;=\; -\vec{\sigma}\,\cdot\,\vec{p}\,P_0\;. \tag{5.18}
$$

Because of the result (5.4) for the small component χ, one can conclude that χ and φ have to have a different parity.

Next we consider the invariance structure of the Hamiltonian and determine the constants of motion. One obtains for the parity operator P

$$
[H, P] \;=\; 0 \tag{5.19}
$$

and with

$$
\begin{aligned}
J \;=\; L \;+\; S \;&=\; \vec{r}\times\vec{p} \;+\; \frac{1}{2}\gamma^5\vec{\alpha} \\
&=\; \vec{r}\times\vec{p} \;+\; \frac{1}{2}\begin{pmatrix} \vec{\sigma} & 0 \\ 0 & \vec{\sigma} \end{pmatrix} \\
&=\; (\vec{r}\times\vec{p} \;+\; \frac{1}{2}\,\vec{\sigma})\;\mathbf{1} \qquad (5.20)
\end{aligned}
$$

one can show that

$$
\begin{aligned}
\left[H, J^2\right] \;&=\; 0 \qquad (5.21) \\
[H, J_3] \;&=\; 0\;.
\end{aligned}
$$

This means we have to determine simultaneous eigenfunctions to $J^2, J_3, \mathbf{P}$ with quantum numbers J, M, ϵ, where

$$
\epsilon \;=\; \begin{cases} +1 & \text{for states with parity} \quad (-1)^{J+\,\frac{1}{2}} \\ -1 & \text{for states with parity} \quad (-1)^{J-\,\frac{1}{2}} \end{cases} \qquad (5.22)
$$

This means explicitly for the states ψ:

$$
\begin{aligned}
J^2\begin{pmatrix}\varphi\\ \chi\end{pmatrix} \;&=\; J(J\;+\;1)\begin{pmatrix}\varphi\\ \chi\end{pmatrix} \qquad (5.23) \\
J_3\begin{pmatrix}\varphi\\ \chi\end{pmatrix} \;&=\; M\begin{pmatrix}\varphi\\ \chi\end{pmatrix} \\
P_0\begin{pmatrix}\varphi\\ \chi\end{pmatrix} \;&=\; (-1)^{J+\,\frac{\epsilon}{2}}\begin{pmatrix}\varphi\\ -\chi\end{pmatrix} \\
P\begin{pmatrix}\varphi\\ \chi\end{pmatrix} \;&=\; (-1)^{J+\,\frac{\epsilon}{2}}\begin{pmatrix}\varphi\\ \chi\end{pmatrix}
\end{aligned}
$$

where $P \;=\; \beta\; P_0$.

Functions which fulfill the properties of (5.24) are the spherical harmonics for the total angular momentum $J, \mathbf{Y}_{LS}^{JM}(\theta, \varphi, S)$. Starting with $Y_{LM_L}(\hat{r}) \;=\; \langle \hat{r} \mid LM_L\rangle$, one obtains

$$
\begin{aligned}
\mathbf{Y}_{LS}^{JM_3}(\hat{r}) \;=\; \langle \hat{r} \mid LSJM_J\rangle \;&=\; \sum_{M_L M_S} \langle \hat{r} \mid LS\; M_S M_L\rangle\langle LS\; M_S M_L \mid LSJ\; M_J\rangle \qquad (5.24) \\
&=\; \sum_{M_L M_S} \langle LS\; M_S M_L \mid LS\; J\; M_J\rangle\; Y_{LM_L}(\hat{r}) \mid SM_S\rangle\;.
\end{aligned}
$$

Considering the action of P_0 on the spherical harmonics

$$P_0 \mathbf{Y}_L^{JM} \;=\; (-1)^L \, \mathbf{Y}_L^{JM} \tag{5.25}$$

with $L_\pm \;:=\; J \;\pm\; \frac{1}{2}$, one sees that $\mathbf{Y}_{L_+}^{JM}$ and $\mathbf{Y}_{L_-}^{JM}$ have different parities.

$$\begin{aligned} P_0 \; \mathbf{Y}_{L_+}^{JM} \;&=\; (-1)^{J+\,\frac{\epsilon}{2}} \, \mathbf{Y}_{L_+}^{JM} \\ P_) \; \mathbf{Y}_{L_-}^{JM} \;&=\; (-1)^{J-\,\frac{\epsilon}{2}} \, \mathbf{Y}_{L_-}^{JM} \;=\; (-1)^{J+\,\frac{\epsilon}{2}} \, (-\mathbf{Y}_{L_-}^{JM}) \; . \end{aligned} \tag{5.26}$$

Knowing that φ and χ from (5.14) must have different parities, we can make the ansatz

$$\begin{aligned} \varphi \;&=\; \frac{F(r)}{r} \, \mathbf{Y}_{L_+}^{JM} \, (\Omega) \\ \chi \;&=\; i \, \frac{G(r)}{r} \, \mathbf{Y}_{L_-}^{JM} \, (\Omega) \; . \end{aligned} \tag{5.27}$$

Here $F(r)$ and $G(r)$ are functions of r, the angle dependence is combined in the spherical harmonics. Thus, for the wave function we obtain

$$\psi_\epsilon^{JM} \;\equiv\; \frac{1}{r} \begin{pmatrix} F(r) & \mathbf{Y}_{L_+}^{JM}(\Omega) \\ iG(r) & \mathbf{Y}_{L_-}^{JM}(\Omega) \end{pmatrix} \; . \tag{5.28}$$

5.3 Determination of the Radial Equation

In order to derive a radial equation, we first need to consider the separation of $\vec{\alpha} \cdot \vec{p}$ into a radial and angular part. Define

$$\alpha_r \;:=\; \vec{\alpha} \;\cdot\; \frac{\vec{r}}{r} \;=\; \frac{\vec{\alpha} \;\cdot\; \vec{r}}{r} \; . \tag{5.29}$$

Thus

$$
\begin{aligned}
P_r &:= \frac{1}{2}\left(\vec{p}\,\cdot\,\frac{\vec{r}}{r} \;+\; \frac{\vec{r}}{r}\,\vec{p}\right) \\
&= \frac{1}{2}\left[\frac{(\vec{p}\cdot\vec{r})}{r} \;+\; \left(\vec{p}\,\frac{1}{r}\right) \;+\; 2\,\frac{\vec{r}}{r}\,\cdot\,\vec{p}\right] \\
&= \frac{1}{2}\left[\frac{3}{ir} \;-\; \frac{1}{ir} \;+\; 2\,\frac{\vec{r}\cdot\vec{p}}{r}\right] \\
&= \frac{1}{r}\left[\frac{1}{r} \;+\; \vec{r}\,\vec{p}\right] \\
&:= \frac{1}{ir}\,\frac{\partial}{\partial r}\,r
\end{aligned}
\tag{5.30}
$$

Now consider

$$
\begin{aligned}
(\vec{\alpha}\cdot\vec{r})(\vec{\alpha}\cdot\vec{p}) &= \begin{pmatrix} \vec{\sigma}\cdot\vec{r}\vec{\sigma}\cdot\vec{p} & 0 \\ 0 & \vec{\sigma}\cdot\vec{r}\vec{\sigma}\cdot\vec{p} \end{pmatrix} \\
&= (\vec{\sigma}\cdot\vec{r}\;\vec{\sigma}\cdot\vec{p})\;\mathbf{1} \\
&= (\vec{r}\cdot\vec{p} \;+\; i\vec{\sigma}\cdot\;\vec{r}\times\vec{p})\;\mathbf{1} \\
&= (\vec{r}\cdot\vec{p} \;+\; i\vec{\sigma}\cdot\vec{L})\;\mathbf{1} \\
&= (rp_r \;+\; i(1 \;+\; \vec{\sigma}\cdot\vec{L}))\;\mathbf{1}\;.
\end{aligned}
\tag{5.31}
$$

Combining (5.31) and (5.32) gives

$$
\frac{\alpha_r}{r}\,(\vec{\alpha}\cdot\vec{r})(\vec{\alpha}\cdot p) \;=\; \frac{(\vec{\alpha}\cdot\vec{r})^2}{r}\,(\vec{\alpha}\cdot\vec{p}) \;=\; \mathbf{1}\,(\vec{\alpha}\cdot\vec{p})
\tag{5.32}
$$

and thus an expression for $\vec{\alpha}\cdot\vec{p}$ in terms of radial quantities

$$
\vec{\alpha}\cdot\vec{p} \;=\; \alpha_r\,\left[p_r \;+\; \frac{i}{r}\,(1 \;+\; \vec{\sigma}\;\cdot\;\vec{L})\right]\;.
\tag{5.33}
$$

We now consider the operation $(1 \;+\; \vec{\sigma}\cdot\vec{L})\;\mathbf{1}$, which gives

$$
(1 \;+\; \vec{\sigma}\cdot\vec{L})\;\mathbf{1} \;\;=\;\; \mathbf{1} \;+\; \begin{pmatrix} \vec{\sigma}\cdot\vec{L} & 0 \\ 0 & \vec{\sigma}\cdot\vec{L} \end{pmatrix}
\tag{5.34}
$$

$$= \mathbf{1} + 2\vec{S} \cdot \vec{L}$$
$$= \mathbf{1} + J^2 - L^2 - S^2$$
$$= J^2 - L^2 + \frac{1}{4} .$$

The operation of L^2 on the Dirac spinor ψ is given as

$$
\begin{aligned}
L^2 \begin{pmatrix} \varphi \\ \chi \end{pmatrix} &= \begin{pmatrix} L_+(L_+ + 1)\ \varphi \\ L_-(L_- + 1)\ \chi \end{pmatrix} \\
&= \begin{pmatrix} \left(J + \frac{\epsilon}{2}\right)\left(J + \frac{\epsilon}{2} + 1\right)\ \varphi \\ \left(J - \frac{\epsilon}{2}\right)\left(J - \frac{\epsilon}{2} + 1\right)\ \chi \end{pmatrix} \\
&= \left(J + \beta\ \frac{\epsilon}{2}\right)\ \left(J + \beta\ \frac{\epsilon}{2} + 1\right)\ \begin{pmatrix} \varphi \\ \chi \end{pmatrix} \\
&= \left[J(J+1) + \frac{1}{4} + \frac{\epsilon}{2}\ (2J+1)\ \beta\right]\ \begin{pmatrix} \varphi \\ \chi \end{pmatrix} .
\end{aligned}
\tag{5.35}
$$

Combining (5.35) and (5.36) leads to

$$(1 + \vec{\sigma} \cdot \vec{L})\ \mathbf{Y}_\epsilon^{JM} = -\frac{\epsilon}{2}\ (2J+1)\ \beta\ \mathbf{Y}_\epsilon^{JM} . \tag{5.36}$$

One now obtains the radial equation by combining (5.33) with (5.36) and (5.9) as

$$\left[\alpha_r\ \left(p_r - \frac{i\epsilon}{r}(J + \frac{1}{2})\ \beta\right) + m\beta + V - E\right]\ \psi_\epsilon^{JM} = 0 . \tag{5.37}$$

Now consider the action of

$$\alpha_r := \frac{\vec{\alpha} \cdot \vec{r}}{r} = \begin{pmatrix} 0 & \frac{\vec{\sigma}\cdot\vec{r}}{r} \\ \frac{\vec{\sigma}\cdot\vec{r}}{r} & 0 \end{pmatrix} \tag{5.38}$$

on the angular function. Consider

$$P_0 \, \frac{\vec{\sigma}\cdot\vec{r}}{r} \, \mathbf{Y}^{JM}_{L_\pm} \;=\; - \, \frac{\vec{\sigma}\cdot\vec{r}}{r} \, P_0 \, \mathbf{Y}^{JM}_{L_\pm} \;=\; - \, \frac{\vec{\sigma}\cdot\vec{r}}{r} \, (-1)^{L_\pm} \, \mathbf{Y}^{JM}_{L_\pm} \;=\; (-1)^{J \mp \frac{\epsilon}{2}} \, \frac{\vec{\sigma}\cdot\vec{r}}{r} \, \mathbf{Y}^{JM}_{L_\pm} \qquad (5.39)$$

where $L_\pm \;=\; J \;\pm\; \frac{\epsilon}{2}$ was used

From (5.40) follows that $\frac{\vec{\sigma}\cdot\vec{r}}{r} \, \mathbf{Y}^{JM}_{L_\pm}$ is eigenfunction of P with eigenvalue $(-1)^{J \mp \frac{\epsilon}{2}}$. Thus

$$\frac{\vec{\sigma}\cdot\vec{r}}{r} \, \mathbf{Y}^{JM}_{L_\pm} \;=\; \text{const} \; \mathbf{Y}^{JM}_{L_\mp} \; . \qquad (5.40)$$

With

$$\left(\frac{\vec{\sigma}\cdot\vec{r}}{r} \right)^2 \;=\; \frac{\vec{r}\cdot\vec{r}}{r^2} \;+\; i \, \vec{\sigma}\cdot\vec{r}\times\vec{r}/r^2 \;=\; 1 \; . \qquad (5.41)$$

We have then

$$\begin{aligned} \alpha_r \; \psi^{JM}_\epsilon \;&=\; \begin{pmatrix} 0 & \frac{\vec{\sigma}\cdot\vec{r}}{r} \\ \frac{\vec{\sigma}\cdot\vec{r}}{r} & 0 \end{pmatrix} \begin{pmatrix} \frac{F}{r} & \mathbf{Y}^{JM}_{L_+} \\ \frac{iG}{r} & \mathbf{Y}^{JM}_{L_-} \end{pmatrix} \;=\; \begin{pmatrix} \pm \, \frac{iG}{r} & \mathbf{Y}^{JM}_{L_+} \\ \pm \, \frac{F}{r} & \mathbf{Y}^{JM}_{L_-} \end{pmatrix} \\ \beta \; \psi^{JM}_\epsilon \;&=\; \begin{pmatrix} \frac{F}{r} & \mathbf{Y}^{JM}_{L_+} \\ - \, \frac{iG}{r} & \mathbf{Y}^{JM}_{L_-} \end{pmatrix} \\ \alpha_r \; \beta \; \psi^{JM}_\epsilon \;&=\; \begin{pmatrix} \mp \, \frac{iG}{r} & \mathbf{Y}^{JM}_{L_+} \\ \pm \, \frac{F}{r} & \mathbf{Y}^{JM}_{L_-} \end{pmatrix} \; . \end{aligned} \qquad (5.42)$$

With this and (5.31) for P_r the radial equations (5.36) takes the form

$$\begin{aligned} \pm \quad \frac{1}{ir} \, \frac{d}{dr} \, r \, \frac{iG}{r} \;\pm\; \frac{i\epsilon}{r} \, \left(J + \frac{1}{2} \right) \, \frac{iG}{r} + (m + V - E) \, \frac{F}{r} \;&=\; 0 \\ \pm \;\; \frac{1}{ir} \, \frac{d}{dr} r \, \frac{F}{r} \;\mp\; \frac{i\epsilon}{r} \, \left(J + \frac{1}{2} \right) \, \frac{F}{r} + \; (-m + V - E) \, \frac{iG}{r} \;&=\; 0 \; . \end{aligned} \qquad (5.43)$$

Multiplying the first equation with r and the second with $\frac{r}{i}$ leads to

$$\pm \; \frac{d}{dr} G \mp \frac{\epsilon}{r} \left(J + \frac{1}{2}\right) G + (V - E + m) F = 0 \qquad (5.44)$$
$$\mp \; \frac{d}{dr} F \mp \mp \frac{\epsilon}{r} \left(J + \frac{1}{2}\right) F + (V - E - m) G = 0$$

or

$$\pm \left[\frac{d}{dr} - \frac{\epsilon}{r} \left(J + \frac{1}{2}\right)\right] G = (E - V - m) F \qquad (5.45)$$
$$\mp \left[- \frac{d}{dr} - \frac{\epsilon}{r} \left(J + \frac{1}{2}\right)\right] F = (E - V + m) G \,.$$

The $E - m$ in (5.46) is the familiar binding energy $-E_B$ (negative for bound states) and $V(r)$) the time-like component of a four-vector potential. The equations (5.46) are highly symmetrical, with the main difference being that F (which is "large" in the non-relativistic limit) is multiplied by the small number $(E - V - m)$, while G (small) is multiplied by a big number $(E - V + m)$.

According to (5.9) the Hamiltonian was given by $H = \vec{\alpha} \cdot \vec{p} + \beta m + V(r)$, where $V(r)$ is a central potential. One can also choose

$$V(r) = \beta \, U(r) \qquad (5.46)$$

where $U(r)$ is a central potential. Then the Hamiltonian is given by

$$H = \vec{\alpha} \cdot \vec{p} + \beta(m + U(r)) \,. \qquad (5.47)$$

The corresponding radial equation is then given by

$$\left[\alpha_r \left(p_r - \frac{i\epsilon}{r} \left(J + \frac{1}{2}\right) \beta\right) + \beta(m + U(r)) - E\right] \psi_\epsilon^{JM} = 0 \,. \qquad (5.48)$$

Inserting

$$\psi_\epsilon^{JM} = \frac{1}{r} \begin{pmatrix} F(r) & \mathbf{Y}_{L_+}^{JM} & (\Omega) \\ iG(r) & \mathbf{Y}_{L_-}^{JM} & (\Omega) \end{pmatrix} \qquad (5.49)$$

gives together with $k = \epsilon\left(J + \frac{1}{2}\right)$

$$\begin{aligned} \pm \frac{d}{dr} G(r) \mp \frac{k}{r} G(r) + (m + U - E) F(r) &= 0 \\ \mp \frac{d}{dr} F(r) \mp \frac{k}{r} F(r) - (m + U + E) G(r) &= 0 . \end{aligned} \tag{5.50}$$

As an aside, choosing $i\psi_\epsilon^{JM}$ instead of (5.49) leads to the same equation (5.51). Conventionally one chooses the "+" for the large component $F(r)$.

Often one takes as most general form of the potential

$$\hat{V}(r) = V(r) + \beta U(r) \tag{5.51}$$

so that the Hamiltonian reads

$$H = \vec{\alpha} \cdot \vec{p} + \beta (m + U(r)) + V(r) . \tag{5.52}$$

5.4 Boundary Conditions for the Radial Functions $F(r)$ and $G(r)$

The full solution ψ_ϵ^{JM} has to be regular at the origin, i.e., at $r = 0$. Thus one has to have

$$F(0) = G(0) = 0 . \tag{5.53}$$

For a potential $V(r) \approx \frac{1}{r}$, the radial equations (5.46) become for $r \to \infty$

$$-\frac{d}{dr} G(r) - (E - m) F(r) = 0 \tag{5.54}$$

$$\frac{d}{dr} F(r) - (E + m) G(r) = 0 . \tag{5.55}$$

From (5.55) follows

$$\frac{d^2}{dr^2} F(r) \; - \; (E+m) \, \frac{d}{dr} \, G(r) \; = \; 0 \tag{5.56}$$

and thus

$$G' \; = \; \frac{1}{E+m} \, F'' \; . \tag{5.57}$$

Inserting (5.57) into (5.54) leads to

$$\begin{aligned} F'' \; &+ \; (E^2 \; - \; m^2) \, F \; = \; 0 \\ F'' \; &- \; (m^2 \; - \; E^2) \, F \; = \; 0 \\ F'' \; &- \; K^2 \, F \; = \; 0 \end{aligned} \tag{5.58}$$

where $K^2 \; = \; m^2 \; - \; E^2$ and $\mid m \mid > E$. From (5.59) one can deduce the behavior of F for $r \to \infty$

$$F(r) \; = \; a \, e^{-Kr} \; . \tag{5.59}$$

From (5.55) follows for $G(r)$:

$$\begin{aligned} G \; &= \; \frac{1}{E+m} \, F' \\ &= \; -a \, \frac{\sqrt{m^2 - E^2}}{E+m} \, e^{-Kr} \\ &= \; -a \, \sqrt{\frac{m-E}{m+E}} \, e^{-Kr} \; . \end{aligned} \tag{5.60}$$

This means that $F(r)$ and G(r) have the same asymptotic behavior for $r \to \infty$.

5.5 The Hydrogen Atom

We now solve the radial equations (5.46) for the Coulomb potential

$$V(r) \;=\; \frac{Ze^2}{r} \; . \tag{5.61}$$

To achieve a simpler form of the equations, we introduce new variables:

$$\begin{aligned}
\kappa &:= \sqrt{m^2 - E^2} \quad \text{with} \quad |\, m \,| \geq E \\
\nu &:= \sqrt{\frac{m - E}{m + E}} \\
\xi &:= Z\, e^2 \\
\tau &:= \epsilon \left(J + \frac{1}{2} \right) \\
\rho &:= kr \; .
\end{aligned} \tag{5.62}$$

With the variables given in (5.63), the radial equations (5.46) take the form

$$\begin{aligned}
\left[\frac{d}{d\rho} - \frac{\tau}{\rho} \right] G &= \left[-\nu + \frac{\xi}{\rho} \right] F \\
- \left[\frac{d}{d\rho} + \frac{\tau}{\rho} \right] F &= \left[\frac{1}{\nu} + \frac{\xi}{\rho} \right] G \; .
\end{aligned} \tag{5.63}$$

For the solution of (5.64) we choose the following ansatz:

$$\begin{aligned}
F(\rho) &= \rho^s \, e^{-\rho} \sum_{k=0}^{\infty} a_k \rho^k \\
G(\rho) &= \rho^s \, e^{-\rho} \sum_{k=0}^{\infty} b_k \rho^k
\end{aligned} \tag{5.64}$$

where $a_0 \neq 0$ and $b_0 \neq 0$.

Taking the derivations with respect to ρ leads to:

$$\frac{d}{d\rho} F(\rho) \;=\; \rho^s \, e^{-\rho} \left[s \, a_0 \, \rho^{-1} + \sum_{k=0}^{\infty} \{ (s + k + 1) \, a_{k+1} - a_k \} \; \rho^k \right] \tag{5.65}$$

$$\begin{aligned}
\frac{d}{d\rho}\, g(\rho) &= \rho^s\, e^{-\rho} \left[s\, b_0\, \rho^{-1} + \sum_{k=0}^{\infty} \{ (s + k + 1)\, b_{k+1} - b_k \}\, \rho^k \right] \\
\frac{1}{\rho}\, F(\rho) &= \rho^s\, e^{-\rho} \left[a_0\, \rho^{-1} + \sum_{k=0}^{\infty} a_{k+1}\, \rho^k \right] \\
\frac{1}{\rho}\, G(\rho) &= \rho^s\, e^{-\rho} \left[b_0\, \rho^{-1} + \sum_{k=0}^{\infty} b_{k+1}\, \rho^k \right] .
\end{aligned}$$

Insertion of (5.64) into the first equation of (5.64) leads to the following condition for the coefficients:

$$(sb_0 - \tau b_0 - \xi a_0)\, \rho^{-1} + \sum_{k=0}^{\infty} \{ (s + k + 1 + \tau)\, b_{k+1} - b_k - \xi\, a_{k+1} + \nu\, a_k \}\, \rho^k = 0\,. \tag{5.66}$$

Insertion into the second equation of (5.64) gives

$$(-sa_0 - \tau a_0 - \xi b_0)\, \rho^{-1} + \sum_{k=0}^{\infty} \left\{ -(s + k + 1 + \tau)\, a_{k+1} + a_k - \frac{1}{\nu}\, b_k - \xi\, b_{k+1} \right\} \rho^k = 0 \tag{5.67}$$

so that both equations (5.66) are fulfilled, the coefficients of ρ have to vanish term by term, i.e.,

$$\begin{aligned}
(s + k + 1 - \tau)\, b_{k+1} - b_k + \nu a_k - \xi a_{k+1} &= 0 \\
-(s + k + 1 + \tau)\, a_{k+1} + a_k - \frac{1}{\nu}\, b_k - \xi b_{k+1} &= 0
\end{aligned} \tag{5.68}$$

for $k = -1, 0, 1, 2, \ldots$ and $b_{-1} = a_{-1} = 0$. Multiplying the second equation in (5.69) with ν and subtracting the equations gives

$$(s + k + 1 - \tau + \nu\xi)\, b_{k+1} + [\nu(s + k = 1 + \tau) - \xi]\, a_{k+1} = 0\,. \tag{5.69}$$

The expansions for $F(r)$ and $G(r)$ are only then finite, if there exists $a_{k'}$ with $a_{k'+1} = b_{k'+1} = 0$ and $a_{k'} \neq 0$ and $b_{k'} \neq 0$.

Let $b_{k'} = \nu a_k$ and $k' = k+1$ and insert into (5.69). This gives the condition for stopping the expansion

$$2(s + k') = \left(\frac{1}{\nu} - \nu\right) \xi \tag{5.70}$$
$$= \left(\sqrt{\frac{m+E}{m-E}} - \sqrt{\frac{m-E}{m+E}}\right) \xi$$
$$= \frac{2E}{\sqrt{m^2 - E^2}} \xi .$$

Thus one obtains

$$(s + k') \sqrt{m^2 - E^2} = E\xi \tag{5.71}$$

from which follows for E

$$E = \frac{m}{\sqrt{1 + \frac{\xi^2}{(s+k')^2)}}} \tag{5.72}$$

s can be obtained from the two recursion formulae (5.69) for the case $k = -1$:

$$(s - \tau) b_0 - \xi a_0 = 0 \tag{5.73}$$
$$-(s + \tau) a_0 - \xi b_0 = 0 .$$

Obtaining b_0 from the first equation and inserting it into the second equation leads to

$$s = \pm \sqrt{\tau^2 - \xi^2} \tag{5.74}$$

so that $F(r)$ and $G(r)$ are regular at $\rho = 0$ (i.e., $F(0) = G(0) = 0$) a necessary and sufficient condition is that

$$s = \sqrt{\tau^2 - \xi^2} . \tag{5.75}$$

With (5.75) one obtains for (5.72)

$$E = \frac{m}{\sqrt{1 + \frac{\xi^2}{k'^2 \sqrt{\tau^2 - \xi^2}}}} . \tag{5.76}$$

With $k' := n - \left(J + \frac{1}{2}\right) = 0, 1, 2, \ldots \infty$, where $n = 1, 2, \ldots \infty$ being the principal quantum number, and

$$\begin{aligned} 0 \leq J + \frac{1}{2} &\leq n \\ 0 \leq L &\leq n - 1 \end{aligned} \tag{5.77}$$

one obtains as final expression for the energy

$$E_{nJ} = \frac{m}{\sqrt{1 + \frac{Z^2 e^4}{\left(n - \left(J + \frac{1}{2}\right) + \sqrt{\left(J + \frac{1}{2}\right)^2 - Z^2 e^4}\right)^2}}} . \tag{5.78}$$

For each k' there exist regular solutions for $\epsilon = +1$ and $\epsilon = -1$. For $n = 1$ there exist only one solution for $\epsilon = -1$.

The expansion of E_{nJ} from (5.78) according to powers of $Z^2 e^4$ gives

$$E_{nJ} = m \left[1 - \frac{Z^2 e^4}{2n^2} - \frac{(Z^2 e^4)^2}{2n^4} \left(\frac{n}{J + \frac{1}{2}} - \frac{3}{4} \right) + \ldots \right] . \tag{5.79}$$

Here m is the mass term. The second term

$$\frac{-m\ Z^2 e^4}{2n^2} \tag{5.80}$$

gives the non-relativistic levels, where n corresponds to the usual principal quantum number.

The term

$$-m\ \frac{(Z^2 e^4)^2}{2n^4} \left(\frac{n}{J + \frac{1}{2}} - \frac{3}{4} \right) \tag{5.81}$$

corresponds to the first relativistic correction and the fine structure splitting. It removes the degeneracy of the non-relativistic levels with respect to n. For a fixed n the binding energy $m - E$ increases with increasing J. The increase depends on J. This means the $L - S$ coupling distinguishes between $J = L \pm \frac{1}{2}$.

The next correction would be the Lamb shift (correction due to the self-energy-radiation of the field). The Lamb shift removes the degeneracy for fixed n and $J = L + \frac{1}{2}$ ($J = (l+1) - \frac{1}{2}$). The next level of corrections is the hyperfine splitting, which give a doublet splitting of all lines and results from the interaction of the proton and the electron.

5.6 The General Force Problem

So far, we solve the Dirac equation for potentials, such as the Coulomb potential, that transform like the time component of a four-vector. Basically, the interaction was introduced via the "minimal coupling" scheme $\partial^\mu \longrightarrow \partial^\mu + iqA^\mu$, or equivalently $p^\mu \to p^\mu - qA^\mu$. The same scheme could have been used to include the space-like parts $\vec{A}$. More general (but still local) potential couplings produce a Dirac equation with the Hamiltonian form

$$i\frac{\partial}{\partial t}\psi(\vec{r},t) + \left(\vec{\alpha}\cdot\frac{\vec{\nabla}}{i} + \beta\left[m + V^s(r) + \gamma^5 V^{ps}(r) + \gamma^\mu V^\nu_\mu(r) + \gamma^\mu\gamma^s V^A_\mu(r) + \sigma^{\mu\nu}V^T_{\mu\nu}(r)\right]\right)\psi(\vec{r},t) = 0 \tag{5.82}$$

Here the subscripts (s, v, ps, A, T) indicate the transformation nature of the potential (scalar, vector, pseudoscalar, axial vector, tensor)[1]. Physically, scalar and pseudoscalar potentials couple to mass, vector and axial vector potentials to four-momenta and tensor potentials to magnetic moments. Because an interaction including all these couplings would not conserve parity, we choose to eliminate the pseudo couplings and consider a simpler version of (5.82)

$$i\,\frac{\partial}{\partial t}\psi(\vec{r},t) = \left(\vec{\alpha}\cdot\frac{\vec{\nabla}}{i} + \beta\left[m + V^s(r) + \gamma^\mu V^V_\mu(r) + \sigma^{\mu\nu}V^T_{\mu\nu}(r)\right]\right)\psi(\vec{r},t) \tag{5.83}$$

[1]Further discussion of solutions to the Dirac equation with these couplings and their phenomenological effects can be found in Clark et al., *Phys. Rev.* **C31**, 694 (1985); ibid: **C31**, 1975 (1985).

5.7 Free Spherical Solutions

For $V(r) = 0$ the radial equations (5.46) take the form

$$\begin{aligned} \pm \left[\frac{d}{dr} - \frac{\epsilon\left(J+\frac{1}{2}\right)}{r}\right] G &= (E-m)\ F \\ \pm \left[-\frac{d}{dr} - \frac{\epsilon\left(J+\frac{1}{2}\right)}{r}\right] F &= (E+m)\ G\ . \end{aligned} \tag{5.84}$$

From the second equation follows

$$G = \frac{\mp 1}{E+m} \left[\frac{d}{dr} + \frac{\epsilon\left(J+\frac{1}{2}\right)}{r}\right] F. \tag{5.85}$$

Inserting (5.85) into the first equation of (5.85) leads to

$$\begin{aligned} \pm\left[\frac{d}{dr} - \frac{\epsilon\left(J+\frac{1}{2}\right)}{r}\right] \frac{(\mp 1)}{(E+m)} \left[\frac{d}{dr} + \frac{\epsilon\left(J+\frac{1}{2}\right)}{r}\right] F &= (E-m)F \\ \left[\frac{d}{dr} - \frac{\epsilon\left(J+\frac{1}{2}\right)}{r}\right] \left[\frac{d}{dr} + \frac{\epsilon\left(J+\frac{1}{2}\right)}{r}\right] F &= -(E^2-m^2)F \\ \left[\frac{d^2}{dr^2} + \frac{d}{dr}\left(\frac{\epsilon\left(J+\frac{1}{2}\right)}{r}\right) - \frac{\epsilon\left(J+\frac{1}{2}\right)}{r}\frac{d}{dr} - \frac{\left(J+\frac{1}{2}\right)^2}{r^2}\right] F &= -(E^2-m^2)F \\ \left[\frac{d^2}{dr^2} - \frac{\epsilon\left(J+\frac{1}{2}\right)}{r^2} - \frac{\left(J+\frac{1}{2}\right)^2}{r^2}\right] F &= -(E^2-m^2)F. \end{aligned} \tag{5.86}$$

The terms $\approx \frac{1}{r^2}$ leads to $-\frac{1}{r^2}\left(J+\frac{1}{2}\right)\left(J+\frac{1}{2}+\epsilon\right) = -\frac{1}{r^2}\ L_+\ (L_+ + 1)$. With $k^2 = E^2 - m^2$, eq. (5.86) takes the form

$$\left[\frac{d^2}{dr^2} - \frac{L_+(L_+ + 1)}{r^2} + k^2\right]\ F\ =\ 0\ . \tag{5.87}$$

For $\epsilon = 1 \Rightarrow L = J - \frac{1}{2}$, and $L_+ = J + \frac{\epsilon}{2}$. Eq. (5.87) has the regular solutions

$$F(r) \;=\; r\, j_{L_+}\,(kr)\;. \tag{5.88}$$

Setting $x \equiv kr$ one has the following relations

$$\begin{aligned} j_{L-1} + j_{L+1} &= \frac{2L+1}{x}\, j_k \\ j_l' &= \frac{1}{2L+1}\,\left(L j_{L-1} - (L+1)\; j_{L+1}\right)\;. \end{aligned} \tag{5.89}$$

From this follows

$$\begin{aligned} x\; j_L' &= \{x\; j_{L-1} - (L+1)\; j_L\} \\ &\qquad -x\; j_{L+1} + L\; j_L\;. \end{aligned} \tag{5.90}$$

Inserting (5.88) into the second equation of (5.85), one obtains a solution for $G(r)$:

$$\begin{aligned} G &= \mp \frac{1}{E+m}\left[\frac{d}{dr} + \frac{\epsilon\left(J+\frac{1}{2}\right)}{r}\right]\; r\; j_L\;(kr) \\ &= \mp \frac{1}{E+m}\left[j_L + kr\; j_L' \;+\; \left\{\begin{array}{c} L \\ -(L+1) \end{array}\right\}\; j_L\right] \\ &= \mp \frac{1}{E+m}\left\{\begin{array}{c} x\; j_{L-1} \\ -x\; j_{L+1} \end{array}\right\} \\ &= \mp \frac{\epsilon k}{E+m}\; r\; j_{L-\epsilon}(kr)\;. \end{aligned} \tag{5.91}$$

One has

$$L \;-\; \epsilon \;=\; \left\{\begin{array}{l} L-1 \;=\; J - \frac{1}{2} \\ L+1 \;= J + \frac{1}{2} \end{array}\right. \tag{5.92}$$

From this follows for $G(r)$

$$G(r) \;=\; \mp\, \frac{\epsilon k}{E+m}\; r\; j_{L_-}\;(kr) \tag{5.93}$$

With

$$\frac{k}{E+m} = \left(\frac{E^2-m^2}{(E+m)^2}\right)^{\frac{1}{2}} = \sqrt{\frac{E-m}{E+m}} \tag{5.94}$$

and

$$\mathbf{Y}^{JM}_{L_-} = \pm\, \vec{\sigma}\cdot\hat{r}\; \mathbf{Y}^{JM}_{L_+} \tag{5.95}$$

one obtains for the free solution of the Dirac equation

$$\psi^{JM}_{\epsilon} = \text{const} \times \begin{pmatrix} \sqrt{E+m}\; j_{L_+}\,(kr) \\ -i\epsilon\,\sqrt{E-m}\; j_{L_-}(kr)\;\vec{\sigma}\;\cdot\;\hat{r} \end{pmatrix} \mathbf{Y}^{JM}_{L_+}\;. \tag{5.96}$$

Let $L_+ = J + \frac{\epsilon}{2} = 0$ then $J = \frac{-\epsilon}{2} \geq 0 \Rightarrow \epsilon = -1 \Rightarrow J = \frac{1}{2}$. Then

$$\begin{aligned} \mathbf{Y}^{\frac{1}{2}\;M}_{o} &= \sum_{M_s} \langle 0\;\frac{1}{2},\;0\;M_s\;\mid \frac{1}{2}M\rangle\;\frac{1}{\sqrt{4\pi}}\;\mid \frac{1}{2}M_s\rangle \\ &= \langle 0\;\frac{1}{2}0M \mid \frac{1}{2}M\rangle \mid \frac{1}{2}M\rangle \\ &= \mid \frac{1}{2}M_s\rangle\;. \end{aligned} \tag{5.97}$$

Thus for $L_+ = 0$ one obtains

$$\psi = N \begin{pmatrix} i\sqrt{E+m}\; j_0(kr) \\ -\sqrt{E-m}\; j_1(kr)\;\vec{\sigma}\cdot\hat{r} \end{pmatrix} \mid \frac{1}{2}\;M_s\rangle \tag{5.98}$$

with

$$\begin{aligned} \frac{1}{N^2} &= \int_V d^3r \langle\;\frac{1}{2}M_s \mid (-i\;\sqrt{E+m}\;j_0, -\sqrt{E-m}\;j_1\;\vec{\sigma}\cdot\hat{r}) \\ &\times \begin{pmatrix} i\sqrt{E+m}\;j_0 \\ -\sqrt{E-m}\;j_1\;\vec{\sigma}\cdot\hat{r} \end{pmatrix} \mid \frac{1}{2}M_s\rangle \\ &= \int_V d^3r\;\langle\frac{1}{2}\;M_s\;\mid (E+m)\;j_0^2\;+\;(E-m)\;j_1^2\;\mid\;\frac{1}{2}\;M_s\rangle \\ &= \int_V d^3r\left[(E+m)j_0^2\;+\;(E-m)j_1^2\right] \end{aligned} \tag{5.99}$$

Let V be a sphere, i.e., $V \equiv V_{sphere} = \frac{4\pi}{3}\ R^2$. Then

$$\begin{aligned}
\frac{1}{N_R^2} &= \frac{1}{k^3} \int_V d^3x \ \left[(E+m)\ j_0^2(x) + \ (E-m)\ j_1^2(x)\right] \qquad (5.100) \\
&= \frac{4\pi}{k^3} \left\{(E+m) \int_0^{kr} dx\ x^2\ j_0^2(x)\ +\ (E-m)\ \int_0^{kr}\ dx\ x^2\ j_1^2(x)\right\} \\
&= \frac{4\pi}{k^3} \left\{(E+m) \frac{1}{2} x^3 \left[j_0^2(x) + n_0(x) j_1(x)\right] + (E-m) \frac{1}{2} x^3 \left[j_1^2(x) - j_0(x) j_2(x)\right]\right\}_0^{kR} \\
&= 2\pi R^3 \left\{2E \left[j_0^2(kR) + j_1^2(kR) - \frac{2}{kR} j_0(kR) j_1(kR)\right] + \frac{2m}{kR} j_0(kR) j_1(kR)\right\}\ .
\end{aligned}$$