On the relativistic $L - S$ coupling

P Alberto, M Fiolhais and M Oliveira
Departamento de Física, Universidade de Coimbra, P-3000 Coimbra, Portugal

Abstract. The fact that the Dirac equation is linear in the space and time derivatives leads to the coupling of spin and orbital angular momenta that is of a pure relativistic nature. We illustrate this fact by computing the solutions of the Dirac equation in an infinite spherical well, which allows to go from the relativistic to the non-relativistic limit by just varying the radius of the well.

PACS numbers: 03.56.Pm, 03.65.Ge

Submitted to: Europ. J. Phys.

1. Introduction

The effect of spin-orbit coupling is well known from elementary quantum mechanics and atomic physics: it arises from the interaction between the spin of an electron in an atom and the magnetic field created by the orbiting nucleus in the rest frame of the electron. This magnetic field is related to the electric field created by the nucleus in its rest frame. If this field is a spherical electrostatic field, the interaction hamiltonian is given by

$$H_{\text{spin-orbit}} = \frac{e}{2m^2c^2} \frac{1}{r} \frac{dV}{dr} \vec{S} \cdot \vec{L}. \tag{1}$$

Here, as usual, $\vec{S}$ and $\vec{L}$ are the spin and orbital momentum operators for the electron, $m$ and $e$ stand for the electron charge and mass, $c$ is the speed of light in the vacuum and $V(r)$ is the electrostatic potential of the atomic nucleus. For one-electron atom, the formula (1) is exact, otherwise $V(r)$ can be thought as an approximation to an average radial potential experienced by the electron. Equation (1) is obtained in the non-relativistic limit (electron velocity is small compared to $c$ — see, for instance, [1]) and so it is used in the non-relativistic description of an electron, i.e., by adding it to the Hamiltonian in the Schrödinger equation.

In this paper we propose to examine a similar coupling that arises due to the relativistic treatment of the electron (i.e. using the Dirac equation) even in the absence of an external field. This is a consequence of the linearity of the Dirac equation in the space derivatives (and thus in the linear momentum operator $\vec{p}$) and from the related fact that one needs a 4-component spinor to describe the electron. We will make the relativistic nature of this coupling apparent by solving the Dirac equation...
in an infinite spherical potential well. Although the particle motion inside the well is free, the relativistic \( L - S \) coupling exists and vanishes only in the non-relativistic limit, which we are able to approach continuously by varying the well radius. In this limit the two-component spinor description is valid.

A comparison between relativistic and non-relativistic solutions was already studied in \[2\] for a one-dimensional infinite square well potential. In the present paper we use the same procedures as in \[2\] to provide a bridge between known relativistic and non-relativistic solutions in the 3-dimensional spherical case, with special emphasis on the \( L - S \) coupling. Berry and Mondragon \[3\] have also applied similar methods in the framework of the Dirac equation in two spatial dimensions.

In section 2 we pedagogically review the solutions of the free Dirac equation with spherical symmetry, in a slightly different fashion from the usual treatments, emphasizing the role of the \( L - S \) coupling term and its consequences for the set of quantum numbers of the solution. In section 3 we solve the Dirac equation for a spherical potential well and compare it to the non-relativistic solution of the corresponding Schrödinger equation for several well radii. Technical details, included for completeness, are mostly left to Appendices.

2. Solutions of the free Dirac equation with spherical symmetry

The free Dirac equation for a spin-\( \frac{1}{2} \) particle with mass \( m \) is a matrix equation for 4-component spinors \( \Psi \) given by

\[
i \hbar \frac{\partial \Psi}{\partial t} = \vec{\alpha} \cdot \vec{p} c \Psi + \beta mc^2 \Psi
\]

where \( \vec{p} = -i \hbar \vec{\nabla} \) is the linear momentum operator, and \( \vec{\alpha} \) and \( \beta \), in the usual representation, are the \( 4 \times 4 \) matrices

\[
\vec{\alpha} = \begin{pmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}.
\]

Here \( I \) is the \( 2 \times 2 \) unit matrix and \( \vec{\sigma} \) denotes the three Pauli matrices \( \sigma_i \quad i = 1, 2, 3 \) obeying the relations

\[
\sigma_i \sigma_j = \delta_{ij} + i \varepsilon_{ijk} \sigma_k \quad i, j = 1, 2, 3
\]

where \( \varepsilon_{ijk} \) is the anti-symmetric Levi-Civita tensor (\( \varepsilon_{123} = 1 \)) and summation over repeated indexes is implied.

Using (4) we can obtain the following general property of the \( \alpha \) matrices

\[
\vec{\alpha} \cdot \vec{A} \vec{\alpha} \cdot \vec{B} = \vec{A} \cdot \vec{B} + i \vec{A} \times \vec{B} \cdot \vec{\Sigma},
\]

where \( \vec{A} \) and \( \vec{B} \) are two arbitrary vectors whose components commute with the matrices \( \alpha_i \) and

\[
\vec{\Sigma} = \begin{pmatrix} \vec{\sigma} & 0 \\ 0 & \vec{\sigma} \end{pmatrix}.
\]
On the relativistic $L - S$ coupling

is the 4-dimensional analog of the Pauli matrices. Using (5) and $\vec{\alpha} \cdot \hat{r} \vec{\alpha} \cdot \hat{r} = I$ (here, of course, $I$ stands for the $4 \times 4$ unit matrix), one can write

$$\vec{\alpha} \cdot \vec{p} = \vec{\alpha} \cdot \hat{r} \vec{\alpha} \cdot \hat{r} \vec{\alpha} \cdot \vec{p}$$

$$= \vec{\alpha} \cdot \hat{r} (\hat{r} \cdot \vec{p} + i \hat{r} \times \vec{p} \cdot \vec{\Sigma})$$

$$= \vec{\alpha} \cdot \hat{r} (\hat{r} \cdot \vec{p} + \frac{i}{r} \vec{L} \cdot \vec{\Sigma}) ,$$

(6)

where $r = |\vec{r}|$, $\hat{r} = \vec{r}/r$ and $\vec{L} = \vec{r} \times \vec{p}$ is the orbital angular momentum operator. Inserting (6) into the Dirac equation (2) we get

$$i \hbar \frac{\partial \Psi}{\partial t} = \vec{\alpha} \cdot \hat{r} (\hat{r} \cdot \vec{p} + \frac{i}{r} \vec{L} \cdot \vec{\Sigma}) c \Psi + \beta mc^2 \Psi .$$

(7)

Since the spin angular momentum operator in the Dirac formalism is $\vec{S} = \frac{\hbar}{2} \vec{\Sigma}$ the last expression contains a term involving the dot product $\vec{L} \cdot \vec{S}$ as in the spin-orbit term (4). This term is responsible for the $L - S$ coupling for a relativistic spin-$\frac{1}{2}$ particle even in the absence of an external potential. Clearly this fact is connected to the spinor structure of the wave function for spin-$\frac{1}{2}$ particles and to the linearity of the Dirac equation, which leads to the appearance of the term $\vec{\alpha} \cdot \vec{p}$. In the Klein-Gordon equation, which is quadratic in the space derivatives, there is no such coupling.

We can gain further insight into the origin of this effect if we write the spinor $\Psi$ in (4) as a set of two-component spinors $\chi'$ and $\varphi'$:

$$\Psi = \begin{pmatrix} \chi' \\ \varphi' \end{pmatrix} .$$

(8)

From the block off-diagonal form of the $\alpha_i$ matrices one sees that the term $\vec{\alpha} \cdot \vec{p}$ mixes the spinors $\chi'$ and $\varphi'$. In the literature (see, for instance, Bjorken and Drell [4]) this kind of term is referred to as “odd” as opposed to the terms like $\beta mc^2$ which are called “even”, since they don’t mix upper and lower two-component spinors. This distinction is important when one goes to the non-relativistic limit of the Dirac equation using the Foldy-Wouthuysen transformation [4 5] which aims at eliminating the odd terms through a unitary transformation and so decouple the upper and lower spinors. In this way one can regain the (Pauli) non-relativistic description of a spin-$\frac{1}{2}$ particle. The fact that the term responsible for the $L - S$ coupling is odd indicates that this relativistic effect is related to the four-component spinor structure, i.e., to the existence of two non-zero spinor components $\chi'$ and $\varphi'$ of the wave function. This will be shown in the following.

Let us consider the stationary solutions of the Dirac equation by writing the spinor $\Psi$ in the form

$$\Psi = e^{-iE/\hbar t} \begin{pmatrix} \chi \\ \varphi \end{pmatrix} ,$$

(9)

‡ We prefer to use this name because there is no orbital motion for a free particle
where $E$ is the total (kinetic plus rest) energy of the fermion. Inserting this expression into (9) we get two equations for the spinors $\varphi$ and $\chi$

\begin{align}
(E - mc^2)\chi &= \vec{\sigma} \cdot \hat{r} (\hat{r} \cdot \vec{p} + \frac{i}{r} \vec{L} \cdot \vec{\sigma}) c \varphi \\
(E + mc^2)\varphi &= \vec{\sigma} \cdot \hat{r} (\hat{r} \cdot \vec{p} + \frac{i}{r} \vec{L} \cdot \vec{\sigma}) c \chi.
\end{align}

From these equations the $L - S$ coupling of the spinors $\varphi$ and $\chi$ becomes apparent. Let us consider solutions with spherical symmetry of these equations. In Appendix A a derivation slightly different from the one used in most textbooks is presented. It is shown that the spinors can be written as products of a radial and an angular function as

\begin{align}
\chi &= i G_{j\ell}(r) \Phi_{j\ell m}(\theta, \phi), \\
\varphi &= -F_{j'\ell'}(r) \Phi_{j'\ell' m}(\theta, \phi) = F_{j'\ell'}(r) \vec{\sigma} \cdot \hat{r} \Phi_{j\ell m},
\end{align}

where $\ell' = \ell - \kappa/|\kappa|$, $\kappa$ being a non-zero quantum number which has a different sign according to the way the spin couples to the orbital angular momentum (see (A.3)). Since $\ell' \neq \ell$ the whole spinor $\Psi$ is not an eigenstate of the orbital angular momentum operator $\vec{L}^2$. The good quantum numbers are $j$ (total angular momentum quantum number), $s = \frac{1}{2}$, $m$ (see Appendix A) and parity. This is due to the $L - S$ term mentioned above.

It is interesting to look at the non-relativistic limit of the equation (11). If we divide it by $mc^2$, we obtain

\begin{equation}
\left( \frac{E}{mc^2} + 1 \right) \varphi = \frac{1}{mc} \vec{\sigma} \cdot \vec{p} \chi,
\end{equation}

using the fact that $\vec{\sigma} \cdot \hat{r} (\hat{r} \cdot \vec{p} + \frac{i}{r} \vec{L} \cdot \vec{\sigma}) c = \vec{\sigma} \cdot \vec{p} c$. In the non-relativistic limit, the linear momenta of the dominant plane-wave components of $\chi$ (obtained through a Fourier decomposition) are much smaller than $mc$, which implies, from (14), that $\varphi$ disappears in that limit. Since the angular part of $\varphi$ contains only geometrical information, we can conclude (see equation (13)) that $F_{j'\ell'}$ vanishes in the non-relativistic limit and one recovers the two-component spinor description of a spin-$\frac{1}{2}$ particle.

Interestingly enough, in the ultra-relativistic limit, where $E + mc^2 \sim E - mc^2 \sim E$, we can again recover the two-component description, since in this case we can choose the spinors $\chi$ and $\varphi$ to be eigenstates of the helicity operator

$$
\vec{\sigma} \cdot \vec{p} c \over E = \vec{\sigma} \cdot \hat{p},
$$

where $\hat{p} = \vec{p}/|\vec{p}|$, with eigenvalues $\pm 1$, as can be seen from equations (10) and (11). This implies that $\chi = \pm \varphi$ and therefore we may construct two two-component spinors for each value of the helicity (see, for instance, Itzykson and Zuber [6]).

If we differentiate once the coupled first order differential equations for $G_{j\ell}$ and $F_{j'\ell'}$ derived in Appendix A (equations (A.11) and (A.12)), one gets

\begin{equation}
\frac{d^2 G_{j\ell}}{dr^2} + 2 \frac{dG_{j\ell}}{dr} - \frac{\ell(\ell + 1)}{r^2} G_{j\ell} + \frac{E^2 - m^2 c^4}{(hc)^2} G_{j\ell} = 0
\end{equation}
On the relativistic $L - S$ coupling

\[
\frac{d^2 F_{j\ell}}{dr^2} + 2 \frac{dF_{j\ell}}{dr} - \frac{\ell' (\ell' + 1)}{r^2} F_{j\ell} + \frac{E^2 - m^2 c^4}{(\hbar c)^2} F_{j\ell} = 0. \tag{16}
\]

Notice that, although in each equation only $\ell$ or $\ell'$ appear explicitly, the radial functions depend also on $j$ through the energy $E$. These are the differential equations which have to be solved in order to get the radial functions $G_{j\ell}$ and $F_{j\ell'}$.

In the non-relativistic limit, since $F_{j\ell'}$ vanishes, $\ell$ is again a good quantum number, i.e., the $L - S$ coupling disappears. Moreover, since in this case $G_{j\ell}$ only depends on $\ell$, we can construct the standard non-relativistic solution taking the linear combination

\[
G_\ell \sum_j \langle \ell m | j m \rangle \Phi_{j\ell m} = G_\ell Y_{\ell m} \chi_m,
\]

where we dropped the index $j$ in the radial function and used the definition (A.1) of $\Phi_{j\ell m}$ and an orthogonality property of the Clebsch-Gordan coefficients.

The differential equations (A.11) and (A.12) can be extended to include interactions with spherical external potentials $V(r)$ and $m(r)$, which are respectively a time component of a four-vector (affecting the energy) and a Lorentz scalar (affecting the mass). This is done by the replacements $E \rightarrow E - V(r)$ and $m \rightarrow m(r)$.

3. Solution of the Dirac equation in an infinite spherical well

In order to show numerically the relativistic nature of the $L - S$ coupling described in the preceding section, we are going now to compute the positive energy solutions of the Dirac equation for an infinite spherical well. As we will show, we can go, in a natural way, from a relativistic to a non-relativistic situation by changing the radius of the potential. The boundary conditions at the wall of the potential provide a discrete energy spectrum which allows a clear picture of the non-relativistic limit.

To solve the Dirac equation in such a potential, one has to avoid any complications due to the negative energy states when trying to localize a spin-$\frac{1}{2}$ particle within a distance of the order of its Compton wavelength $\hbar/(mc)$ or less (this is the case for confined relativistic particles), one example of which is the Klein paradox (see, for instance, [4]). In other words, we want to retain the rôle of the Dirac equation as a one-particle equation in the presence of a infinite external potential. This is accomplished by defining a Lorentz scalar potential, i.e., a mass-like potential, having the form

\[
m(r) = \begin{cases} 
m & r < R \\
\infty & r > R
\end{cases},
\]

where $m$ is the mass of the particle. The effect of this potential is to prevent the particle from propagating outside the well, meaning that its wave function is identically zero there. Inside, it behaves as a free particle of mass $m$. A potential like (18), usually with $m = 0$, has been used to describe confined quarks as constituents of the nucleon in the MIT bag model (see, e.g., [8] for a review of this and related models).

The boundary condition for the wave function at the boundary ($r = R$) cannot be obtained by requiring its continuity, since, being the Dirac equation a first-order
differential equation, the potential \( [13] \) implies that there is an infinite jump in the derivative of \( \Psi \) (i.e., in the radial derivatives of \( G \) and \( F \)) when the boundary of the well is crossed. This jump obviously would not exist if \( \Psi \) were continuous. Another and most natural alternative is to demand that the probability current flux at the boundary is zero. As it is shown in \([3]\), this is also a necessary condition to assure the hermiticity of the kinetic part of the Dirac hamiltonian within the well. This can be achieved by the condition

\[
-i \beta \vec{a} \cdot \vec{r} \Psi = \Psi \quad \text{at} \quad r = R. \tag{19}
\]

In fact, if one multiplies this equation on the left by \( \Psi^{\dagger} \beta \) and its hermitian conjugate on the right by \( \beta \Psi \) one gets \(-i \Psi^{\dagger} \alpha \cdot \vec{r} \Psi = \Psi^{\dagger} \beta \Psi \) and \(-i \Psi^{\dagger} \alpha \cdot \vec{r} \Psi = \Psi^{\dagger} \beta \Psi \) at \( r = R \). These two equations imply that \( \Psi^{\dagger} \beta \Psi \) and \( \Psi^{\dagger} \alpha \cdot \vec{r} \Psi \) are zero at \( r = R \).

The expression \( \Psi^{\dagger} \alpha \cdot \vec{r} \Psi \) can also be written as \( \vec{j} \cdot \vec{r} / c \), where \( \vec{j} = \Psi^{\dagger} \alpha \Psi c \) is the probability current density for the particle described by the wave function \( \Psi \). Instead of the current flux we can look at the value of \( \Psi^{\dagger} \beta \Psi \) at the boundary: indeed, since \( \Psi \) is zero for \( r > R \), we may as well summarize the effect of the boundary condition \([19]\) by saying that \( \Psi^{\dagger} \beta \Psi \) is continuous for any value of \( r \).

Having established the boundary condition, we proceed now to compute the radial functions. This is done in Appendix C. The full spinor \( \Psi \) reads

\[
\Psi_{jkm}(r, \theta, \phi, t) = A e^{-iE/\hbar t} \left( i j_\ell \left( \frac{\sqrt{E^2 - mc^2}}{hc} r \right) \Phi_{j\ell m}(\theta, \phi) - \frac{\kappa}{|\kappa|} \sqrt{\frac{E - mc^2}{E + mc^2}} j_\ell \left( \frac{\sqrt{E^2 - mc^2}}{hc} r \right) \Phi_{j\ell ' m}(\theta, \phi) \right) , \tag{20}
\]

where \( A \) is determined from normalization. In order to obtain the energy spectrum, we apply the boundary condition \([19]\) to the spinor \([20]\). This gives rise to an equation relating the two radial functions (see Appendix C)

\[
j_\ell(X) = -\frac{\kappa}{|\kappa|} \sqrt{\frac{E - mc^2}{E + mc^2}} j_\ell'(X) \tag{21}
\]

where \( X = \sqrt{E^2 - mc^2} / (hc) R \). It can be written, in a more convenient way, in terms of the scaled quantities \( y = (E - mc^2) / (mc^2) \) and \( x_R = R / L_0 \), with \( L_0 = \hbar / (mc) \). These are the kinetic energy in units of \( mc^2 \) and the well radius in units of the Compton wavelength, respectively. We get then

\[
j_\ell(x_R \sqrt{y^2 + 2y}) = -\frac{\kappa}{|\kappa|} \sqrt{\frac{y}{y + 2}} j_\ell'(x_R \sqrt{y^2 + 2y}) . \tag{22}
\]

This equation is solved numerically for \( y \) as a function of \( x_R \) for a given set of \( \ell, \ell' \) and \( \kappa \). The results are presented in Figure 1. We plot the first values of \( y \) up to \( \ell = 5 \) for three values of \( x_R \). The energy levels are labeled in standard spectroscopic notation \( n \ell_j \), where \( n \) denotes the \( n \)th solution for a given set of \( \ell \) and \( j \). For \( x_R = 100 \) the non-relativistic results, using the notation \( n \ell \), are also presented. The non-relativistic spectrum is obtained by solving the Schrödinger equation for a particle of mass \( m \) in an infinite spherical potential well of radius \( R = 100 L_0 \). The solutions can be found, for instance, in the quantum mechanics textbook of Landau \([10]\) (in this case, there is no
spin-orbit coupling of the type (II) because the potential is zero inside the well). The radial functions are spherical Bessel functions subject to the boundary condition

$$j_\ell(kR) = 0, \quad k = \frac{\sqrt{2mE_k}}{\hbar},$$

(23)

where $E_k$ is the kinetic energy of the particle. Notice that, in the non-relativistic limit, $y \ll 1$, equation (22) reduces to (23) since

$$x_R \sqrt{y^2 + 2y} \sim x_R \sqrt{2y} = \frac{\sqrt{2mE_k}}{\hbar} R,$$

(24)

and the factor $\sqrt{y/(y + 2)}$ goes to zero in this limit.

Analyzing Figure 1, we see that, as the radius of the well increases, the energy levels with the same $\ell$ start grouping until they become degenerate and almost identical to the corresponding non-relativistic values. This effect is more pronounced for the states with higher $\ell$ (notice the behaviour of the $1h_{9/2}$ and $1h_{11/2}$ states). So we can conclude...
that going from a radius \( R = L_0 \) to a radius \( R = 100L_0 \) the \( L - S \) coupling effect fades away and \( j \) is no longer needed to classify the eigenstates of the system, and instead the orbital momentum quantum number \( \ell \) emerges as the relevant quantum number. Since the boundary condition \([22]\) effectively imposes a (maximum) value for the wavelength of the wave function and thereby a (minimum) value for the energy through the De Broglie relation, increasing the radius of the well amounts to decreasing the energy until we reach non-relativistic values for \( R = 100L_0 \). Notice that for the higher levels, for this value of \( R \), even though there is not a perfect match with the non-relativistic energy values, the vanishing of the \( L - S \) coupling is a fact. The crucial scale here is the Compton wavelength \( L_0 = \frac{\hbar}{mc} \), determining the relativistic nature of the solution through the well radius.

In summary, we have showed numerically the relativistic nature of the \( L - S \) coupling in the Dirac equation by computing its solutions for a particle with mass \( m \) in an infinite spherical potential well of radius \( R \) and making \( R \) sufficiently big as to produce non-relativistic solutions.

Acknowledgments

This work was supported by the Project PRAXIS/PCEX/C/FIS/6/96.

Appendix A.

In this Appendix the radial equations for the Dirac equation are derived. We first write \( \varphi \) and \( \chi \) in equations (10) and (11) as products of a radial function and a function of the angular coordinates \( \theta \) and \( \phi \). To be able to get ordinary differential equations for the radial functions, the angular function must be an eigenstate of the operator \( \vec{L} \cdot \vec{\sigma} = \left( \vec{J}^2 - \vec{L}^2 - \vec{S}^2 \right)/\hbar \) (where \( \vec{J} = \vec{L} + \vec{S} \) denotes the total angular momentum), which acts only on the angular coordinates. Accordingly, the angular function, \( \Phi_{j\ell m} \), reads

\[
\Phi_{j\ell m}(\theta, \phi) = \sum_{m_s=-\ell}^{\ell} \langle \ell m_s | j m \rangle Y_{\ell m_s}(\theta, \phi) \chi_{m_s}
\]

where \( Y_{\ell m_s}(\theta, \phi) \) is the spherical harmonic with quantum numbers \( \ell \) and \( m_s \), \( \chi_{m_s} \) the two-component spinors

\[
\chi_{\frac{\ell}{2}} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \chi_{-\frac{\ell}{2}} = \begin{pmatrix} 0 \\ 1 \end{pmatrix},
\]

and \( \langle \ell m_s | j m \rangle \) is a Clebsch-Gordan coefficient. The wave function \((A.1)\) is an eigenstate of \( \frac{1}{2} \vec{L}^2 \), \( \vec{J}^2 \), \( \vec{S}^2 \) and \( J_z \) with eigenvalues \( \hbar^2 j(j+1) \), \( \hbar^2 \ell(\ell+1) \), \( \hbar^2 \left( \frac{1}{2} + 1 \right) = \hbar^2 \frac{3}{4} \) and \( \hbar m \) respectively. Therefore we have

\[
\vec{L} \cdot \vec{\sigma} \Phi_{j\ell m} = \hbar[j(j+1) + \ell(\ell+1) - 3/4] \Phi_{j\ell m} = -\hbar(1 + \kappa) \Phi_{j\ell m}
\]

\[
(A.2)
\]
with
\[
\kappa = \begin{cases} 
-(\ell + 1) = -(j + \frac{1}{2}) & j = \ell + \frac{1}{2} \\
\ell = j + \frac{1}{2} & j = \ell - \frac{1}{2}.
\end{cases}
\] (A.3)

For a fixed \( j \), the quantum number \( \kappa \) takes into account the two different possibilities
for \( \ell \), namely \( \ell = j \pm \frac{1}{2} \), by just changing its sign. It also satisfies the equality
\( \kappa(\kappa + 1) = \ell(\ell + 1) \) for a certain \( \ell \). Thus \( \kappa \) can be considered
as an alternative quantum number for the wave function \( \Phi_{j\ell m} \) replacing \( \ell \). The corresponding operator
is \(-(\hat{h} + \vec{L} \cdot \vec{\sigma})\). Note that for \( \ell = 0 \) only one value of \( \kappa \) is defined \((-1)\). Wave functions
with a fixed \( j \) but different \( \ell 's \) have opposite parity, since \( \ell = j \pm \frac{1}{2} \) and parity is given
by \((-1)^{\ell} \). Using standard notation, \( \varphi \) and \( \chi \) are then written as
\[
\chi = i G_{j\ell}(r)\Phi_{j\ell m}(\theta, \phi),
\] (A.4)
\[
\varphi = -F_{j\ell}(r)\Phi_{j\ell m}(\theta, \phi).
\] (A.5)

The quantum number \( \ell ' \) of the lower component \( \varphi \) can be found by applying the operator
\( \vec{\sigma} \cdot \vec{r}(\vec{r} \cdot \vec{p} + \frac{i}{2} \vec{L} \cdot \vec{\sigma}) \) to \( \chi \) (see equation (11)), giving
\[
\vec{\sigma} \cdot \vec{r}(\vec{r} \cdot \vec{p} + \frac{i}{2} \vec{L} \cdot \vec{\sigma}) c \chi = c \vec{\sigma} \cdot \vec{r}(-i\hbar \frac{\partial}{\partial r} + \frac{i}{r} \vec{L} \cdot \vec{\sigma})i G_{j\ell}(r)\Phi_{j\ell m}
= \hbar c \left[ \frac{dG_{j\ell}}{dr} + (1 + \kappa) \frac{G_{j\ell}}{r} \right] \vec{r} \cdot \hat{r} \Phi_{j\ell m}.
\] (A.6)

The effect of \( \vec{\sigma} \cdot \vec{r} \) over \( \Phi_{j\ell m} \) can be computed using the tensor properties of \( \vec{\sigma} \) and \( \vec{r} \) (see Appendix B), yielding
\[
\vec{\sigma} \cdot \vec{r} \Phi_{j\ell m} = -\Phi_{j\ell m},
\] (A.7)
where \( \ell ' \) is given by
\[
\ell ' = \begin{cases} 
\ell + 1 & \text{if } j = \ell + \frac{1}{2} \\
\ell - 1 & \text{if } j = \ell - \frac{1}{2}.
\end{cases}
\] (A.8)

Note that \( \ell ' \) is related to \( \ell \) by \( \ell ' = \ell - \kappa/|\kappa| \). If we define the operator
\[
K = \begin{pmatrix} 
-(\hbar + \vec{L} \cdot \vec{\sigma}) & 0 \\
0 & \hbar + \vec{L} \cdot \vec{\sigma}
\end{pmatrix},
\] (A.9)
\( \Psi \) will be an eigenstate of \( K \) with eigenvalue \( \kappa \). Thus \( \kappa \) is also a good quantum number.
From (11) and (A.6) we can write \( \varphi \) in (A.3) in the form
\[
\varphi = F_{j\ell}(r) \vec{\sigma} \cdot \vec{r} \Phi_{j\ell m}(\theta, \phi).
\] (A.10)

The radial functions \( G_{j\ell}(r) \) and \( F_{j\ell}(r) \) satisfy the coupled differential equations
(see equations (11) and (11))
\[
(E - mc^2)G_{j\ell} = -\hbar c \left[ \frac{dF_{j\ell}}{dr} + (1 + \kappa) \frac{F_{j\ell}}{r} \right],
\] (A.11)
\[
(E + mc^2)F_{j\ell} = \hbar c \left[ \frac{dG_{j\ell}}{dr} + (1 + \kappa) \frac{G_{j\ell}}{r} \right],
\] (A.12)
where \( \kappa ' \) is related to \( \ell ' \) in the same way as in (A.3) (giving the relation \( \kappa ' = -\kappa \))
and the relation \( \vec{\sigma} \cdot \vec{r} \Phi_{j\ell m} = -\Phi_{j\ell m} \) was used (note that \((\vec{\sigma} \cdot \vec{r})^2 = I)),
Appendix B.

In this Appendix we will derive expression (A.7) by calculating the matrix element
\[ \Phi_j^{\ell m'} \bar{\sigma} \cdot \hat{r} \Phi_{j\ell m} , \]  
where \( \dagger \) stands for the hermitian conjugate. Since both \( \bar{\sigma} \) and \( \hat{r} \) are vector operators (irreducible tensor operators of rank 1) we can use a general theorem for the matrix element of a scalar product of commuting tensor operators between eigenstates of angular momentum. Using the notation and conventions of Edmonds [7] we have
\[ \Phi_j^{\ell m'} \bar{\sigma} \cdot \hat{r} \Phi_{j\ell m} = (-1)^{\ell + \frac{1}{2} + j} \delta_{jj'} \delta_{mm'} \left\{ \frac{1}{2} \langle \bar{\sigma} \| \frac{1}{2} \rangle \langle \ell' \| \hat{r} \| \ell \rangle \right\} . \]  
Using the conventions of Edmonds, the reduced matrix elements can be evaluated, such that
\[ \Phi_j^{\ell m'} \bar{\sigma} \cdot \hat{r} \Phi_{j\ell m} = (-1)^{\ell + \frac{1}{2} + j} \delta_{jj'} \delta_{mm'} \sqrt{6(2\ell + 1)} \langle 10 ; \ell 0 | \ell' 0 \rangle \left\{ \frac{1}{2} \langle \bar{\sigma} \| \frac{1}{2} \rangle \langle \ell' \| \hat{r} \| \ell \rangle \right\} , \]  
where we used the fact that \( \langle 10 ; \ell 0 | \ell' 0 \rangle \) is non-zero only for \( \ell' = \ell \pm 1 \). The 6-\( j \) symbol is different from zero only for \( j = \ell \pm \frac{1}{2} \). Since we have also \( j = \ell \pm \frac{1}{2} \), we have two possibilities for a fixed \( \ell \):

1) \( j = \ell + \frac{1}{2} \quad \Rightarrow \quad \ell' = \ell + 1 ; \ j = \ell - \frac{1}{2} \)  \hfill (B.4)

2) \( j = \ell - \frac{1}{2} \quad \Rightarrow \quad \ell' = \ell - 1 ; \ j = \ell + \frac{1}{2} \)  \hfill (B.5)

Inserting the values of the Clebsch-Gordan coefficient \( \langle 10 ; \ell 0 | \ell' 0 \rangle \) and of the 6-\( j \) symbol into (B.3) we get, for both cases,
\[ \Phi_j^{\ell m'} \bar{\sigma} \cdot \hat{r} \Phi_{j\ell m} = -\delta_{jj'} \delta_{mm'} , \]  
where \( \ell \) and \( \ell' \) are related by (B.4) and (B.5). Since the spinors \( \Phi_{j\ell m} \) form a complete orthonormal set this equation implies (A.7).

Appendix C.

In this Appendix we obtain the spinor which is the solution of the Dirac equation with the infinite spherical potential (18). To compute the radial functions \( G_{j\ell} \) and \( F_{j'\ell'} \) inside the well, we first look at equations (15) and (16) and make the change of variable \( x = \sqrt{E^2 - m^2 c^4/\hbar^2 c^2} \). In this way, we get equations of the form
\[ \frac{d^2 f_l}{dx^2} + \frac{2}{x} \frac{df_l}{dx} + \left( 1 - \frac{l(l+1)}{x^2} \right) f_l = 0 , \]  
where \( l \) and \( f_l \) stand for \( \ell, \ell' \) and \( G_{j\ell}, F_{j'\ell'} \), respectively. The solutions of equation (C.1) which are regular at the origin are the spherical Bessel functions of the first kind, \( j_l(x) \) (see, for instance, Abramowitz and Stegun [9]). Since these solutions are determined up to an arbitrary multiplicative constant, the radial functions are
\[ G_{j\ell} = A j_{j\ell}(x) \]  
\[ F_{j'\ell'} = B j_{j'\ell'}(x) , \]
On the relativistic $L - S$ coupling

where $A$ are $B$ are constants. We can use one of the equations (A.11) or (A.12) and the recurrence relations of the functions $j_l(x)$ (see [9]) to find the following relation:

$$B = A \frac{\kappa}{|\kappa|} \sqrt{\frac{E - mc^2}{E + mc^2}}. \quad (C.4)$$

The complete spinor $\Psi$ then reads

$$\Psi_{j\kappa m}(r, \theta, \phi, t) = A e^{-iE/\hbar t} \left( -\frac{\kappa}{|\kappa|} \sqrt{\frac{E - mc^2}{E + mc^2}} j_{\ell}(X) \Phi_{j\ell m}(\theta, \phi) \right). \quad (C.5)$$

Applying the boundary condition (19) to this spinor leads to

$$\left( -i \frac{\kappa}{|\kappa|} \sqrt{\frac{E - mc^2}{E + mc^2}} j_{\ell}'(X) \Phi_{j\ell m} \right) = \left( -\frac{\kappa}{|\kappa|} \sqrt{\frac{E - mc^2}{E + mc^2}} j_{\ell}'(X) \Phi_{j\ell m} \right), \quad (C.6)$$

where $X = \sqrt{E^2 - m^2c^4}/(\hbar c) R$ and the relation (A.7) and its inverse were used. This equality implies

$$j_{\ell}'(X) = -\frac{\kappa}{|\kappa|} \sqrt{\frac{E - mc^2}{E + mc^2}} j_{\ell}(X) \quad (C.7)$$

References

[1] Bethe A H and Jackiw R 1968 *Intermediate Quantum Mechanics* (Reading: W. A. Benjamin)
[2] Alberto P, Fiolhais C and Gil V M S 1996 *Eur. J. Phys.* 17 19
[3] Berry M V and Mondragon R J 1987 *Proc. R. Soc. Lond.* A412 53
[4] Bjorken J D and Drell S D 1964 *Relativistic Quantum Mechanics* (New York: McGraw-Hill)
[5] Foldy L L and Wouthysen S A 1950 *Phys. Rev.* 78 29
[6] Itzykson C and Zuber J-B 1980 *Quantum Field Theory* (New York: McGraw-Hill)
[7] Edmonds A R 1957 *Angular Momentum in Quantum Mechanics* (Princeton: Princeton University Press)
[8] Thomas A W 1984 *Adv. in Nucl. Phys.* 13 1
[9] Abramowitz M and Stegun I A 1970 *Handbook of Mathematical Functions* (New York: Dover Publ. Inc.)
[10] Landau L and Lifshitz E M 1994 *Quantum mechanics, non-relativistic theory* (Exeter: Pergamon)